FIGURE 1

Table 1 **Coordinate data on the BRC4-RAD51 complex.**

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1 | CB | GLU | A | 98 | 54.122 | 26.467 | 6.057 | 1.00 | 41.21 | A |
| ATOM | 2 | CG | GLU | A | 98 | 55.636 | 26.317 | 6.015 | 1.00 | 45.64 | A |
| ATOM | 3 | CD | GLU | A | 98 | 56.085 | 25.256 | 5.027 | 1.00 | 47.43 | A |
| ATOM | 4 | OE1 | GLU | A | 98 | 55.620 | 24.103 | 5.147 | 1.00 | 49.28 | A |
| ATOM | 5 | OE2 | GLU | A | 98 | 56.901 | 25.572 | 4.134 | 1.00 | 49.29 | A |
| ATOM | 6 | C | GLU | A | 98 | 51.999 | 26.666 | 4.744 | 1.00 | 34.53 | A |
| ATOM | 7 | O | GLU | A | 98 | 51.235 | 27.538 | 5.157 | 1.00 | 34.61 | A |
| ATOM | 8 | N | GLU | A | 98 | 53.866 | 28.288 | 4.399 | 1.00 | 38.15 | A |
| ATOM | 9 | CA | GLU | A | 98 | 53.509 | 26.878 | 4.717 | 1.00 | 37.21 | A |
| ATOM | 10 | N | ILE | A | 99 | 51.587 | 25.484 | 4.306 | 1.00 | 30.62 | A |
| ATOM | 11 | CA | ILE | A | 99 | 50.181 | 25.125 | 4.226 | 1.00 | 26.62 | A |
| ATOM | 12 | CB | ILE | A | 99 | 49.982 | 24.054 | 3.143 | 1.00 | 28.34 | A |
| ATOM | 13 | CG2 | ILE | A | 99 | 48.540 | 23.603 | 3.115 | 1.00 | 29.76 | A |
| ATOM | 14 | CG1 | ILE | A | 99 | 50.421 | 24.613 | 1.790 | 1.00 | 29.12 | A |
| ATOM | 15 | CD1 | ILE | A | 99 | 50.399 | 23.600 | .678 | 1.00 | 33.00 | A |
| ATOM | 16 | C | ILE | A | 99 | 49.542 | 24.625 | 5.516 | 1.00 | 22.96 | A |
| ATOM | 17 | O | ILE | A | 99 | 50.152 | 23.893 | 6.292 | 1.00 | 22.20 | A |
| ATOM | 18 | N | ILE | A | 100 | 48.299 | 25.039 | 5.728 | 1.00 | 19.56 | A |
| ATOM | 19 | CA | ILE | A | 100 | 47.524 | 24.619 | 6.885 | 1.00 | 16.84 | A |
| ATOM | 20 | CB | ILE | A | 100 | 46.967 | 25.825 | 7.679 | 1.00 | 16.90 | A |
| ATOM | 21 | CG2 | ILE | A | 100 | 45.957 | 25.344 | 8.714 | 1.00 | 18.72 | A |
| ATOM | 22 | CG1 | ILE | A | 100 | 48.113 | 26.580 | 8.358 | 1.00 | 19.95 | A |
| ATOM | 23 | CD1 | ILE | A | 100 | 47.669 | 27.845 | 9.089 | 1.00 | 22.55 | A |
| ATOM | 24 | C | ILE | A | 100 | 46.356 | 23.824 | 6.315 | 1.00 | 15.59 | A |
| ATOM | 25 | O | ILE | A | 100 | 45.805 | 24.185 | 5.275 | 1.00 | 14.24 | A |
| ATOM | 26 | N | GLN | A | 101 | 45.999 | 22.731 | 6.978 | 1.00 | 13.53 | A |
| ATOM | 27 | CA | GLN | A | 101 | 44.887 | 21.907 | 6.523 | 1.00 | 15.11 | A |
| ATOM | 28 | CB | GLN | A | 101 | 45.348 | 20.464 | 6.330 | 1.00 | 19.35 | A |
| ATOM | 29 | CG | GLN | A | 101 | 46.592 | 20.374 | 5.458 | 1.00 | 26.50 | A |
| ATOM | 30 | CD | GLN | A | 101 | 46.427 | 19.451 | 4.273 | 1.00 | 31.87 | A |
| ATOM | 31 | OE1 | GLN | A | 101 | 45.487 | 19.588 | 3.488 | 1.00 | 35.05 | A |
| ATOM | 32 | NE2 | GLN | A | 101 | 47.350 | 18.507 | 4.129 | 1.00 | 33.92 | A |
| ATOM | 33 | C | GLN | A | 101 | 43.786 | 21.993 | 7.564 | 1.00 | 13.47 | A |
| ATOM | 34 | O | GLN | A | 101 | 43.959 | 21.568 | 8.706 | 1.00 | 15.75 | A |
| ATOM | 35 | N | ILE | A | 102 | 42.654 | 22.557 | 7.161 | 1.00 | 10.05 | A |
| ATOM | 36 | CA | ILE | A | 102 | 41.520 | 22.748 | 8.060 | 1.00 | 8.05 | A |
| ATOM | 37 | CB | ILE | A | 102 | 40.706 | 23.983 | 7.633 | 1.00 | 8.89 | A |
| ATOM | 38 | CG2 | ILE | A | 102 | 39.544 | 24.206 | 8.599 | 1.00 | 8.83 | A |
| ATOM | 39 | CG1 | ILE | A | 102 | 41.620 | 25.215 | 7.602 | 1.00 | 11.08 | A |
| ATOM | 40 | CD1 | ILE | A | 102 | 41.023 | 26.415 | 6.880 | 1.00 | 9.86 | A |
| ATOM | 41 | C | ILE | A | 102 | 40.604 | 21.531 | 8.085 | 1.00 | 8.43 | A |
| ATOM | 42 | O | ILE | A | 102 | 40.166 | 21.054 | 7.042 | 1.00 | 8.83 | A |
| ATOM | 43 | N | THR | A | 103 | 40.309 | 21.036 | 9.282 | 1.00 | 8.44 | A |
| ATOM | 44 | CA | THR | A | 103 | 39.446 | 19.868 | 9.411 | 1.00 | 9.31 | A |
| ATOM | 45 | CB | THR | A | 103 | 39.386 | 19.368 | 10.872 | 1.00 | 10.02 | A |
| ATOM | 46 | OG1 | THR | A | 103 | 38.605 | 18.164 | 10.929 | 1.00 | 11.79 | A |
| ATOM | 47 | CG2 | THR | A | 103 | 38.755 | 20.417 | 11.776 | 1.00 | 11.70 | A |
| ATOM | 48 | C | THR | A | 103 | 38.020 | 20.116 | 8.923 | 1.00 | 9.93 | A |
| ATOM | 49 | O | THR | A | 103 | 37.449 | 21.186 | 9.141 | 1.00 | 8.54 | A |
| ATOM | 50 | N | THR | A | 104 | 37.456 | 19.110 | 8.259 | 1.00 | 10.38 | A |
| ATOM | 51 | CA | THR | A | 104 | 36.091 | 19.174 | 7.737 | 1.00 | 11.01 | A |
| ATOM | 52 | CB | THR | A | 104 | 35.912 | 18.256 | 6.510 | 1.00 | 11.26 | A |
| ATOM | 53 | OG1 | THR | A | 104 | 36.128 | 16.896 | 6.914 | 1.00 | 14.11 | A |
| ATOM | 54 | CG2 | THR | A | 104 | 36.892 | 18.613 | 5.415 | 1.00 | 12.62 | A |
| ATOM | 55 | C | THR | A | 104 | 35.090 | 18.688 | 8.784 | 1.00 | 11.39 | A |
| ATOM | 56 | O | THR | A | 104 | 33.878 | 18.830 | 8.604 | 1.00 | 12.53 | A |
| ATOM | 57 | N | GLY | A | 105 | 35.598 | 18.109 | 9.868 | 1.00 | 10.65 | A |
| ATOM | 58 | CA | GLY | A | 105 | 34.724 | 17.582 | 10.901 | 1.00 | 11.97 | A |
| ATOM | 59 | C | GLY | A | 105 | 34.619 | 16.071 | 10.780 | 1.00 | 13.09 | A |
| ATOM | 60 | O | GLY | A | 105 | 34.156 | 15.390 | 11.699 | 1.00 | 13.32 | A |
| ATOM | 61 | N | SER | A | 106 | 35.052 | 15.550 | 9.634 | 1.00 | 12.40 | A |
| ATOM | 62 | CA | SER | A | 106 | 35.033 | 14.115 | 9.363 | 1.00 | 14.20 | A |
| ATOM | 63 | CB | SER | A | 106 | 34.242 | 13.835 | 8.079 | 1.00 | 14.61 | A |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 64 | OG | SER | A | 106 | 34.505 | 12.528 | 7.589 | 1.00 | 14.19 | A |
| ATOM | 65 | C | SER | A | 106 | 36.453 | 13.563 | 9.217 | 1.00 | 14.25 | A |
| ATOM | 66 | O | SER | A | 106 | 37.230 | 14.041 | 8.391 | 1.00 | 13.00 | A |
| ATOM | 67 | N | LYS | A | 107 | 36.788 | 12.553 | 10.017 | 1.00 | 15.63 | A |
| ATOM | 68 | CA | LYS | A | 107 | 38.117 | 11.946 | 9.951 | 1.00 | 17.24 | A |
| ATOM | 69 | CB | LYS | A | 107 | 38.279 | 10.867 | 11.026 | 1.00 | 21.76 | A |
| ATOM | 70 | CG | LYS | A | 107 | 38.184 | 11.361 | 12.456 | 1.00 | 26.56 | A |
| ATOM | 71 | CD | LYS | A | 107 | 38.430 | 10.209 | 13.417 | 1.00 | 31.38 | A |
| ATOM | 72 | CE | LYS | A | 107 | 38.312 | 10.642 | 14.868 | 1.00 | 35.03 | A |
| ATOM | 73 | NZ | LYS | A | 107 | 38.599 | 9.505 | 15.791 | 1.00 | 37.82 | A |
| ATOM | 74 | C | LYS | A | 107 | 38.359 | 11.310 | 8.587 | 1.00 | 16.91 | A |
| ATOM | 75 | O | LYS | A | 107 | 39.446 | 11.430 | 8.020 | 1.00 | 16.59 | A |
| ATOM | 76 | N | GLU | A | 108 | 37.345 | 10.623 | 8.068 | 1.00 | 16.08 | A |
| ATOM | 77 | CA | GLU | A | 108 | 37.464 | 9.970 | 6.770 | 1.00 | 16.56 | A |
| ATOM | 78 | CB | GLU | A | 108 | 36.252 | 9.072 | 6.508 | 1.00 | 18.83 | A |
| ATOM | 79 | CG | GLU | A | 108 | 36.214 | 7.829 | 7.379 | 1.00 | 24.11 | A |
| ATOM | 80 | CD | GLU | A | 108 | 37.473 | 6.991 | 7.241 | 1.00 | 29.12 | A |
| ATOM | 81 | OE1 | GLU | A | 108 | 37.798 | 6.583 | 6.104 | 1.00 | 31.85 | A |
| ATOM | 82 | OE2 | GLU | A | 108 | 38.136 | 6.742 | 8.268 | 1.00 | 31.72 | A |
| ATOM | 83 | C | GLU | A | 108 | 37.611 | 10.973 | 5.641 | 1.00 | 14.32 | A |
| ATOM | 84 | O | GLU | A | 108 | 38.403 | 10.768 | 4.720 | 1.00 | 15.54 | A |
| ATOM | 85 | N | LEU | A | 109 | 36.842 | 12.057 | 5.703 | 1.00 | 14.02 | A |
| ATOM | 86 | CA | LEU | A | 109 | 36.920 | 13.072 | 4.667 | 1.00 | 13.21 | A |
| ATOM | 87 | CB | LEU | A | 109 | 35.772 | 14.076 | 4.823 | 1.00 | 14.04 | A |
| ATOM | 88 | CG | LEU | A | 109 | 35.622 | 15.125 | 3.721 | 1.00 | 15.48 | A |
| ATOM | 89 | CD1 | LEU | A | 109 | 35.590 | 14.448 | 2.353 | 1.00 | 17.82 | A |
| ATOM | 90 | CD2 | LEU | A | 109 | 34.345 | 15.925 | 3.958 | 1.00 | 15.78 | A |
| ATOM | 91 | C | LEU | A | 109 | 38.280 | 13.769 | 4.754 | 1.00 | 14.45 | A |
| ATOM | 92 | O | LEU | A | 109 | 38.896 | 14.070 | 3.731 | 1.00 | 15.30 | A |
| ATOM | 93 | N | ASP | A | 110 | 38.751 | 14.014 | 5.977 | 1.00 | 13.76 | A |
| ATOM | 94 | CA | ASP | A | 110 | 40.056 | 14.644 | 6.170 | 1.00 | 14.88 | A |
| ATOM | 95 | CB | ASP | A | 110 | 40.349 | 14.864 | 7.661 | 1.00 | 15.02 | A |
| ATOM | 96 | CG | ASP | A | 110 | 39.606 | 16.057 | 8.240 | 1.00 | 15.43 | A |
| ATOM | 97 | OD1 | ASP | A | 110 | 38.930 | 16.782 | 7.475 | 1.00 | 15.66 | A |
| ATOM | 98 | OD2 | ASP | A | 110 | 39.706 | 16.272 | 9.471 | 1.00 | 15.62 | A |
| ATOM | 99 | C | ASP | A | 110 | 41.152 | 13.762 | 5.566 | 1.00 | 15.86 | A |
| ATOM | 100 | O | ASP | A | 110 | 42.067 | 14.261 | 4.910 | 1.00 | 15.60 | A |
| ATOM | 101 | N | LYS | A | 111 | 41.061 | 12.451 | 5.788 | 1.00 | 17.06 | A |
| ATOM | 102 | CA | LYS | A | 111 | 42.056 | 11.528 | 5.242 | 1.00 | 19.14 | A |
| ATOM | 103 | CB | LYS | A | 111 | 41.773 | 10.094 | 5.692 | 1.00 | 21.83 | A |
| ATOM | 104 | CG | LYS | A | 111 | 41.970 | 9.845 | 7.176 | 1.00 | 28.51 | A |
| ATOM | 105 | CD | LYS | A | 111 | 41.702 | 8.384 | 7.515 | 1.00 | 32.83 | A |
| ATOM | 106 | CE | LYS | A | 111 | 41.819 | 8.123 | 9.007 | 1.00 | 35.12 | A |
| ATOM | 107 | NZ | LYS | A | 111 | 41.489 | 6.707 | 9.342 | 1.00 | 37.22 | A |
| ATOM | 108 | C | LYS | A | 111 | 42.070 | 11.585 | 3.720 | 1.00 | 18.08 | A |
| ATOM | 109 | O | LYS | A | 111 | 43.136 | 11.599 | 3.098 | 1.00 | 19.72 | A |
| ATOM | 110 | N | LEU | A | 112 | 40.885 | 11.616 | 3.119 | 1.00 | 18.52 | A |
| ATOM | 111 | CA | LEU | A | 112 | 40.771 | 11.680 | 1.666 | 1.00 | 18.11 | A |
| ATOM | 112 | CB | LEU | A | 112 | 39.300 | 11.662 | 1.244 | 1.00 | 18.15 | A |
| ATOM | 113 | CG | LEU | A | 112 | 39.045 | 11.712 | -.266 | 1.00 | 19.29 | A |
| ATOM | 114 | CD1 | LEU | A | 112 | 39.575 | 10.438 | -.906 | 1.00 | 20.79 | A |
| ATOM | 115 | CD2 | LEU | A | 112 | 37.556 | 11.857 | -.538 | 1.00 | 18.97 | A |
| ATOM | 116 | C | LEU | A | 112 | 41.424 | 12.958 | 1.151 | 1.00 | 18.62 | A |
| ATOM | 117 | O | LEU | A | 112 | 42.010 | 12.979 | .063 | 1.00 | 18.72 | A |
| ATOM | 118 | N | LEU | A | 113 | 41.315 | 14.021 | 1.944 | 1.00 | 18.70 | A |
| ATOM | 119 | CA | LEU | A | 113 | 41.879 | 15.321 | 1.592 | 1.00 | 18.77 | A |
| ATOM | 120 | CB | LEU | A | 113 | 41.003 | 16.442 | 2.160 | 1.00 | 18.91 | A |
| ATOM | 121 | CG | LEU | A | 113 | 39.611 | 16.587 | 1.546 | 1.00 | 21.50 | A |
| ATOM | 122 | CD1 | LEU | A | 113 | 38.779 | 17.536 | 2.391 | 1.00 | 21.32 | A |
| ATOM | 123 | CD2 | LEU | A | 113 | 39.735 | 17.096 | .120 | 1.00 | 22.16 | A |
| ATOM | 124 | C | LEU | A | 113 | 43.313 | 15.493 | 2.085 | 1.00 | 20.09 | A |
| ATOM | 125 | O | LEU | A | 113 | 43.843 | 16.606 | 2.098 | 1.00 | 20.28 | A |
| ATOM | 126 | N | GLN | A | 114 | 43.935 | 14.392 | 2.498 | 1.00 | 19.91 | A |
| ATOM | 127 | CA | GLN | A | 114 | 45.313 | 14.420 | 2.974 | 1.00 | 21.17 | A |
| ATOM | 128 | CB | GLN | A | 114 | 46.245 | 14.852 | 1.841 | 1.00 | 22.49 | A |
| ATOM | 129 | CG | GLN | A | 114 | 46.229 | 13.937 | .635 | 1.00 | 23.81 | A |
| ATOM | 130 | CD | GLN | A | 114 | 47.072 | 14.475 | -.504 | 1.00 | 24.77 | A |
| ATOM | 131 | OE1 | GLN | A | 114 | 48.272 | 14.698 | -.351 | 1.00 | 27.78 | A |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 132 | NE2 | GLN | A | 114 | 46.444 | 14.691 | -1.653 | 1.00 | 26.62 | A |
| ATOM | 133 | C | GLN | A | 114 | 45.521 | 15.340 | 4.171 | 1.00 | 20.81 | A |
| ATOM | 134 | O | GLN | A | 114 | 46.588 | 15.938 | 4.323 | 1.00 | 24.10 | A |
| ATOM | 135 | N | GLY | A | 115 | 44.506 | 15.455 | 5.019 | 1.00 | 18.52 | A |
| ATOM | 136 | CA | GLY | A | 115 | 44.628 | 16.302 | 6.189 | 1.00 | 19.04 | A |
| ATOM | 137 | C | GLY | A | 115 | 43.440 | 17.215 | 6.393 | 1.00 | 17.02 | A |
| ATOM | 138 | O | GLY | A | 115 | 43.026 | 17.462 | 7.524 | 1.00 | 18.66 | A |
| ATOM | 139 | N | GLY | A | 116 | 42.886 | 17.714 | 5.292 | 1.00 | 15.87 | A |
| ATOM | 140 | CA | GLY | A | 116 | 41.740 | 18.600 | 5.372 | 1.00 | 14.66 | A |
| ATOM | 141 | C | GLY | A | 116 | 41.760 | 19.626 | 4.253 | 1.00 | 14.23 | A |
| ATOM | 142 | O | GLY | A | 116 | 42.488 | 19.462 | 3.276 | 1.00 | 14.98 | A |
| ATOM | 143 | N | ILE | A | 117 | 40.967 | 20.683 | 4.393 | 1.00 | 12.49 | A |
| ATOM | 144 | CA | ILE | A | 117 | 40.907 | 21.738 | 3.384 | 1.00 | 11.37 | A |
| ATOM | 145 | CB | ILE | A | 117 | 39.677 | 22.639 | 3.619 | 1.00 | 10.73 | A |
| ATOM | 146 | CG2 | ILE | A | 117 | 39.706 | 23.836 | 2.676 | 1.00 | 12.58 | A |
| ATOM | 147 | CG1 | ILE | A | 117 | 38.396 | 21.819 | 3.429 | 1.00 | 12.81 | A |
| ATOM | 148 | CD1 | ILE | A | 117 | 38.180 | 21.302 | 2.016 | 1.00 | 14.44 | A |
| ATOM | 149 | C | ILE | A | 117 | 42.195 | 22.559 | 3.428 | 1.00 | 10.95 | A |
| ATOM | 150 | O | ILE | A | 117 | 42.578 | 23.093 | 4.466 | 1.00 | 12.19 | A |
| ATOM | 151 | N | GLU | A | 118 | 42.849 | 22.665 | 2.277 | 1.00 | 10.51 | A |
| ATOM | 152 | CA | GLU | A | 118 | 44.132 | 23.343 | 2.151 | 1.00 | 12.58 | A |
| ATOM | 153 | CB | GLU | A | 118 | 44.870 | 22.714 | .968 | 1.00 | 15.64 | A |
| ATOM | 154 | CG | GLU | A | 118 | 46.365 | 22.783 | 1.022 | 1.00 | 21.41 | A |
| ATOM | 155 | CD | GLU | A | 118 | 46.996 | 21.963 | -.085 | 1.00 | 20.95 | A |
| ATOM | 156 | OE1 | GLU | A | 118 | 47.180 | 22.499 | -1.194 | 1.00 | 23.24 | A |
| ATOM | 157 | OE2 | GLU | A | 118 | 47.284 | 20.773 | .156 | 1.00 | 26.48 | A |
| ATOM | 158 | C | GLU | A | 118 | 44.120 | 24.861 | 1.982 | 1.00 | 12.88 | A |
| ATOM | 159 | O | GLU | A | 118 | 43.449 | 25.384 | 1.098 | 1.00 | 12.57 | A |
| ATOM | 160 | N | THR | A | 119 | 44.872 | 25.569 | 2.822 | 1.00 | 11.45 | A |
| ATOM | 161 | CA | THR | A | 119 | 44.962 | 27.017 | 2.681 | 1.00 | 11.27 | A |
| ATOM | 162 | CB | THR | A | 119 | 45.553 | 27.700 | 3.946 | 1.00 | 11.65 | A |
| ATOM | 163 | OG1 | THR | A | 119 | 46.863 | 27.180 | 4.220 | 1.00 | 12.69 | A |
| ATOM | 164 | CG2 | THR | A | 119 | 44.650 | 27.468 | 5.149 | 1.00 | 11.67 | A |
| ATOM | 165 | C | THR | A | 119 | 45.891 | 27.282 | 1.492 | 1.00 | 11.98 | A |
| ATOM | 166 | O | THR | A | 119 | 46.769 | 26.467 | 1.194 | 1.00 | 12.27 | A |
| ATOM | 167 | N | GLY | A | 120 | 45.679 | 28.397 | .798 | 1.00 | 10.27 | A |
| ATOM | 168 | CA | GLY | A | 120 | 46.526 | 28.740 | -.333 | 1.00 | 10.55 | A |
| ATOM | 169 | C | GLY | A | 120 | 46.071 | 28.245 | -1.690 | 1.00 | 10.39 | A |
| ATOM | 170 | O | GLY | A | 120 | 46.737 | 28.490 | -2.700 | 1.00 | 11.43 | A |
| ATOM | 171 | N | SER | A | 121 | 44.948 | 27.534 | -1.726 | 1.00 | 10.13 | A |
| ATOM | 172 | CA | SER | A | 121 | 44.423 | 27.028 | -2.984 | 1.00 | 9.86 | A |
| ATOM | 173 | CB | SER | A | 121 | 45.008 | 25.645 | -3.299 | 1.00 | 13.87 | A |
| ATOM | 174 | OG | SER | A | 121 | 44.622 | 24.700 | -2.326 | 1.00 | 19.34 | A |
| ATOM | 175 | C | SER | A | 121 | 42.904 | 26.947 | -2.918 | 1.00 | 9.08 | A |
| ATOM | 176 | O | SER | A | 121 | 42.302 | 27.194 | -1.875 | 1.00 | 8.68 | A |
| ATOM | 177 | N | ILE | A | 122 | 42.298 | 26.611 | -4.048 | 1.00 | 9.44 | A |
| ATOM | 178 | CA | ILE | A | 122 | 40.854 | 26.503 | -4.154 | 1.00 | 10.10 | A |
| ATOM | 179 | CB | ILE | A | 122 | 40.360 | 27.090 | -5.505 | 1.00 | 10.40 | A |
| ATOM | 180 | CG2 | ILE | A | 122 | 38.858 | 26.863 | -5.663 | 1.00 | 12.37 | A |
| ATOM | 181 | CG1 | ILE | A | 122 | 40.702 | 28.579 | -5.586 | 1.00 | 13.97 | A |
| ATOM | 182 | CD1 | ILE | A | 122 | 40.453 | 29.187 | -6.952 | 1.00 | 14.82 | A |
| ATOM | 183 | C | ILE | A | 122 | 40.381 | 25.056 | -4.072 | 1.00 | 11.37 | A |
| ATOM | 184 | O | ILE | A | 122 | 40.982 | 24.162 | -4.666 | 1.00 | 12.71 | A |
| ATOM | 185 | N | THR | A | 123 | 39.323 | 24.832 | -3.304 | 1.00 | 9.56 | A |
| ATOM | 186 | CA | THR | A | 123 | 38.708 | 23.513 | -3.212 | 1.00 | 9.79 | A |
| ATOM | 187 | CB | THR | A | 123 | 38.526 | 23.041 | -1.760 | 1.00 | 10.66 | A |
| ATOM | 188 | OG1 | THR | A | 123 | 39.811 | 22.851 | -1.158 | 1.00 | 13.42 | A |
| ATOM | 189 | CG2 | THR | A | 123 | 37.751 | 21.719 | -1.724 | 1.00 | 10.55 | A |
| ATOM | 190 | C | THR | A | 123 | 37.339 | 23.769 | -3.827 | 1.00 | 8.71 | A |
| ATOM | 191 | O | THR | A | 123 | 36.581 | 24.603 | -3.329 | 1.00 | 10.46 | A |
| ATOM | 192 | N | GLU | A | 124 | 37.041 | 23.084 | -4.926 | 1.00 | 9.35 | A |
| ATOM | 193 | CA | GLU | A | 124 | 35.770 | 23.256 | -5.624 | 1.00 | 9.53 | A |
| ATOM | 194 | CB | GLU | A | 124 | 36.043 | 23.472 | -7.115 | 1.00 | 12.39 | A |
| ATOM | 195 | CG | GLU | A | 124 | 34.820 | 23.549 | -8.006 | 1.00 | 13.73 | A |
| ATOM | 196 | CD | GLU | A | 124 | 35.199 | 23.914 | -9.429 | 1.00 | 17.73 | A |
| ATOM | 197 | OE1 | GLU | A | 124 | 36.273 | 23.462 | -9.887 | 1.00 | 16.72 | A |
| ATOM | 198 | OE2 | GLU | A | 124 | 34.428 | 24.647 | -10.086 | 1.00 | 18.68 | A |
| ATOM | 199 | C | GLU | A | 124 | 34.900 | 22.025 | -5.399 | 1.00 | 10.21 | A |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 200 | O | GLU | A | 124 | 35.283 | 20.911 | -5.749 | 1.00 | 10.78 | A |
| ATOM | 201 | N | MSE | A | 125 | 33.729 | 22.239 | -4.807 | 1.00 | 10.59 | A |
| ATOM | 202 | CA | MSE | A | 125 | 32.825 | 21.143 | -4.495 | 1.00 | 11.22 | A |
| ATOM | 203 | CB | MSE | A | 125 | 32.413 | 21.237 | -3.028 | 1.00 | 13.67 | A |
| ATOM | 204 | CG | MSE | A | 125 | 33.605 | 21.453 | -2.110 | 1.00 | 14.05 | A |
| ATOM | 205 | SE | MSE | A | 125 | 33.164 | 21.237 | -.250 | 1.00 | 21.89 | A |
| ATOM | 206 | CE | MSE | A | 125 | 31.991 | 22.745 | -.036 | 1.00 | 16.55 | A |
| ATOM | 207 | C | MSE | A | 125 | 31.595 | 21.128 | -5.387 | 1.00 | 12.28 | A |
| ATOM | 208 | O | MSE | A | 125 | 30.878 | 22.123 | -5.495 | 1.00 | 12.87 | A |
| ATOM | 209 | N | PHE | A | 126 | 31.361 | 19.986 | -6.026 | 1.00 | 13.37 | A |
| ATOM | 210 | CA | PHE | A | 126 | 30.220 | 19.829 | -6.917 | 1.00 | 14.46 | A |
| ATOM | 211 | CB | PHE | A | 126 | 30.634 | 19.085 | -8.185 | 1.00 | 13.72 | A |
| ATOM | 212 | CG | PHE | A | 126 | 31.575 | 19.857 | -9.059 | 1.00 | 15.70 | A |
| ATOM | 213 | CD1 | PHE | A | 126 | 32.938 | 19.890 | -8.783 | 1.00 | 16.05 | A |
| ATOM | 214 | CD2 | PHE | A | 126 | 31.095 | 20.565 | -10.155 | 1.00 | 15.36 | A |
| ATOM | 215 | CE1 | PHE | A | 126 | 33.811 | 20.619 | -9.588 | 1.00 | 16.76 | A |
| ATOM | 216 | CE2 | PHE | A | 126 | 31.961 | 21.297 | -10.966 | 1.00 | 16.46 | A |
| ATOM | 217 | CZ | PHE | A | 126 | 33.320 | 21.323 | -10.682 | 1.00 | 15.73 | A |
| ATOM | 218 | C | PHE | A | 126 | 29.078 | 19.083 | -6.252 | 1.00 | 16.95 | A |
| ATOM | 219 | O | PHE | A | 126 | 29.292 | 18.071 | -5.589 | 1.00 | 16.20 | A |
| ATOM | 220 | N | GLY | A | 127 | 27.866 | 19.597 | -6.442 | 1.00 | 19.76 | A |
| ATOM | 221 | CA | GLY | A | 127 | 26.683 | 18.983 | -5.866 | 1.00 | 22.59 | A |
| ATOM | 222 | C | GLY | A | 127 | 25.608 | 20.006 | -5.542 | 1.00 | 24.79 | A |
| ATOM | 223 | O | GLY | A | 127 | 25.904 | 21.181 | -5.300 | 1.00 | 24.48 | A |
| ATOM | 224 | N | GLU | A | 128 | 24.354 | 19.561 | -5.535 | 1.00 | 27.02 | A |
| ATOM | 225 | CA | GLU | A | 128 | 23.230 | 20.442 | -5.228 | 1.00 | 28.56 | A |
| ATOM | 226 | CB | GLU | A | 128 | 21.929 | 19.863 | -5.787 | 1.00 | 31.81 | A |
| ATOM | 227 | CG | GLU | A | 128 | 21.852 | 19.818 | -7.305 | 1.00 | 36.61 | A |
| ATOM | 228 | CD | GLU | A | 128 | 21.889 | 21.199 | -7.932 | 1.00 | 39.77 | A |
| ATOM | 229 | OE1 | GLU | A | 128 | 21.116 | 22.075 | -7.487 | 1.00 | 42.32 | A |
| ATOM | 230 | OE2 | GLU | A | 128 | 22.685 | 21.410 | -8.874 | 1.00 | 41.49 | A |
| ATOM | 231 | C | GLU | A | 128 | 23.089 | 20.606 | -3.721 | 1.00 | 27.92 | A |
| ATOM | 232 | O | GLU | A | 128 | 23.714 | 19.878 | -2.949 | 1.00 | 27.36 | A |
| ATOM | 233 | N | PHE | A | 129 | 22.269 | 21.567 | -3.306 | 1.00 | 26.59 | A |
| ATOM | 234 | CA | PHE | A | 129 | 22.044 | 21.794 | -1.887 | 1.00 | 26.34 | A |
| ATOM | 235 | CB | PHE | A | 129 | 20.979 | 22.879 | -1.682 | 1.00 | 26.99 | A |
| ATOM | 236 | CG | PHE | A | 129 | 20.628 | 23.128 | -.238 | 1.00 | 27.71 | A |
| ATOM | 237 | CD1 | PHE | A | 129 | 21.607 | 23.501 | .678 | 1.00 | 26.29 | A |
| ATOM | 238 | CD2 | PHE | A | 129 | 19.311 | 23.006 | .203 | 1.00 | 27.59 | A |
| ATOM | 239 | CE1 | PHE | A | 129 | 21.284 | 23.751 | 2.013 | 1.00 | 27.10 | A |
| ATOM | 240 | CE2 | PHE | A | 129 | 18.976 | 23.253 | 1.537 | 1.00 | 27.95 | A |
| ATOM | 241 | CZ | PHE | A | 129 | 19.966 | 23.627 | 2.443 | 1.00 | 28.18 | A |
| ATOM | 242 | C | PHE | A | 129 | 21.567 | 20.467 | -1.312 | 1.00 | 26.38 | A |
| ATOM | 243 | O | PHE | A | 129 | 20.789 | 19.756 | -1.949 | 1.00 | 26.54 | A |
| ATOM | 244 | N | ARG | A | 130 | 22.062 | 20.138 | -.124 | 1.00 | 25.28 | A |
| ATOM | 245 | CA | ARG | A | 130 | 21.727 | 18.909 | .589 | 1.00 | 24.10 | A |
| ATOM | 246 | CB | ARG | A | 130 | 20.270 | 18.507 | .331 | 1.00 | 27.41 | A |
| ATOM | 247 | CG | ARG | A | 130 | 19.291 | 19.529 | .893 | 1.00 | 32.24 | A |
| ATOM | 248 | CD | ARG | A | 130 | 17.866 | 19.017 | .958 | 1.00 | 38.42 | A |
| ATOM | 249 | NE | ARG | A | 130 | 17.058 | 19.876 | 1.820 | 1.00 | 44.65 | A |
| ATOM | 250 | CZ | ARG | A | 130 | 15.787 | 19.650 | 2.135 | 1.00 | 48.26 | A |
| ATOM | 251 | NH1 | ARG | A | 130 | 15.160 | 18.583 | 1.657 | 1.00 | 50.05 | A |
| ATOM | 252 | NH2 | ARG | A | 130 | 15.144 | 20.490 | 2.937 | 1.00 | 49.61 | A |
| ATOM | 253 | C | ARG | A | 130 | 22.666 | 17.735 | .327 | 1.00 | 21.02 | A |
| ATOM | 254 | O | ARG | A | 130 | 22.608 | 16.737 | 1.035 | 1.00 | 20.30 | A |
| ATOM | 255 | N | THR | A | 131 | 23.530 | 17.846 | -.680 | 1.00 | 19.13 | A |
| ATOM | 256 | CA | THR | A | 131 | 24.490 | 16.776 | -.955 | 1.00 | 17.15 | A |
| ATOM | 257 | CB | THR | A | 131 | 25.129 | 16.904 | -2.351 | 1.00 | 19.70 | A |
| ATOM | 258 | OG1 | THR | A | 131 | 25.761 | 18.184 | -2.469 | 1.00 | 21.01 | A |
| ATOM | 259 | CG2 | THR | A | 131 | 24.079 | 16.744 | -3.439 | 1.00 | 22.19 | A |
| ATOM | 260 | C | THR | A | 131 | 25.601 | 16.899 | .082 | 1.00 | 16.43 | A |
| ATOM | 261 | O | THR | A | 131 | 26.455 | 16.020 | .212 | 1.00 | 15.57 | A |
| ATOM | 262 | N | GLY | A | 132 | 25.583 | 18.012 | .810 | 1.00 | 15.23 | A |
| ATOM | 263 | CA | GLY | A | 132 | 26.581 | 18.246 | 1.836 | 1.00 | 14.02 | A |
| ATOM | 264 | C | GLY | A | 132 | 27.459 | 19.463 | 1.598 | 1.00 | 13.72 | A |
| ATOM | 265 | O | GLY | A | 132 | 28.118 | 19.935 | 2.524 | 1.00 | 13.81 | A |
| ATOM | 266 | N | LYS | A | 133 | 27.467 | 19.986 | .374 | 1.00 | 12.58 | A |
| ATOM | 267 | CA | LYS | A | 133 | 28.306 | 21.140 | .060 | 1.00 | 12.45 | A |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 268 | CB | LYS | A | 133 | 28.111 | 21.557 | -1.408 | 1.00 | 13.99 | A |
| ATOM | 269 | CG | LYS | A | 133 | 26.687 | 21.910 | -1.804 | 1.00 | 16.59 | A |
| ATOM | 270 | CD | LYS | A | 133 | 26.511 | 23.414 | -1.951 | 1.00 | 19.12 | A |
| ATOM | 271 | CE | LYS | A | 133 | 25.098 | 23.756 | -2.398 | 1.00 | 21.74 | A |
| ATOM | 272 | NZ | LYS | A | 133 | 24.906 | 25.222 | -2.577 | 1.00 | 23.48 | A |
| ATOM | 273 | C | LYS | A | 133 | 28.111 | 22.343 | .990 | 1.00 | 11.78 | A |
| ATOM | 274 | O | LYS | A | 133 | 29.084 | 22.923 | 1.476 | 1.00 | 12.85 | A |
| ATOM | 275 | N | THR | A | 134 | 26.866 | 22.718 | 1.250 | 1.00 | 12.16 | A |
| ATOM | 276 | CA | THR | A | 134 | 26.615 | 23.856 | 2.123 | 1.00 | 12.03 | A |
| ATOM | 277 | CB | THR | A | 134 | 25.169 | 24.366 | 1.959 | 1.00 | 12.33 | A |
| ATOM | 278 | OG1 | THR | A | 134 | 24.999 | 24.861 | .622 | 1.00 | 14.07 | A |
| ATOM | 279 | CG2 | THR | A | 134 | 24.874 | 25.485 | 2.950 | 1.00 | 14.49 | A |
| ATOM | 280 | C | THR | A | 134 | 26.892 | 23.515 | 3.585 | 1.00 | 11.44 | A |
| ATOM | 281 | O | THR | A | 134 | 27.315 | 24.380 | 4.357 | 1.00 | 11.86 | A |
| ATOM | 282 | N | GLN | A | 135 | 26.668 | 22.260 | 3.964 | 1.00 | 11.19 | A |
| ATOM | 283 | CA | GLN | A | 135 | 26.920 | 21.833 | 5.339 | 1.00 | 9.68 | A |
| ATOM | 284 | CB | GLN | A | 135 | 26.391 | 20.419 | 5.581 | 1.00 | 12.98 | A |
| ATOM | 285 | CG | GLN | A | 135 | 24.923 | 20.247 | 5.243 | 1.00 | 15.40 | A |
| ATOM | 286 | CD | GLN | A | 135 | 24.058 | 21.355 | 5.807 | 1.00 | 19.13 | A |
| ATOM | 287 | OE1 | GLN | A | 135 | 23.318 | 22.011 | 5.071 | 1.00 | 22.64 | A |
| ATOM | 288 | NE2 | GLN | A | 135 | 24.141 | 21.570 | 7.115 | 1.00 | 16.98 | A |
| ATOM | 289 | C | GLN | A | 135 | 28.420 | 21.868 | 5.605 | 1.00 | 10.76 | A |
| ATOM | 290 | O | GLN | A | 135 | 28.859 | 22.279 | 6.679 | 1.00 | 9.99 | A |
| ATOM | 291 | N | ILE | A | 136 | 29.204 | 21.432 | 4.624 | 1.00 | 9.71 | A |
| ATOM | 292 | CA | ILE | A | 136 | 30.655 | 21.449 | 4.761 | 1.00 | 10.04 | A |
| ATOM | 293 | CB | ILE | A | 136 | 31.345 | 20.817 | 3.528 | 1.00 | 9.93 | A |
| ATOM | 294 | CG2 | ILE | A | 136 | 32.840 | 21.125 | 3.548 | 1.00 | 12.14 | A |
| ATOM | 295 | CG1 | ILE | A | 136 | 31.113 | 19.303 | 3.528 | 1.00 | 12.11 | A |
| ATOM | 296 | CD1 | ILE | A | 136 | 31.574 | 18.602 | 2.263 | 1.00 | 10.81 | A |
| ATOM | 297 | C | ILE | A | 136 | 31.112 | 22.896 | 4.924 | 1.00 | 10.64 | A |
| ATOM | 298 | O | ILE | A | 136 | 31.962 | 23.195 | 5.764 | 1.00 | 9.71 | A |
| ATOM | 299 | N | CYS | A | 137 | 30.537 | 23.796 | 4.129 | 1.00 | 10.36 | A |
| ATOM | 300 | CA | CYS | A | 137 | 30.896 | 25.209 | 4.210 | 1.00 | 10.00 | A |
| ATOM | 301 | CB | CYS | A | 137 | 30.135 | 26.025 | 3.164 | 1.00 | 8.86 | A |
| ATOM | 302 | SG | CYS | A | 137 | 30.711 | 25.760 | 1.458 | 1.00 | 13.33 | A |
| ATOM | 303 | C | CYS | A | 137 | 30.620 | 25.777 | 5.598 | 1.00 | 7.98 | A |
| ATOM | 304 | O | CYS | A | 137 | 31.448 | 26.500 | 6.151 | 1.00 | 10.27 | A |
| ATOM | 305 | N | HIS | A | 138 | 29.461 | 25.456 | 6.165 | 1.00 | 8.44 | A |
| ATOM | 306 | CA | HIS | A | 138 | 29.131 | 25.960 | 7.493 | 1.00 | 7.87 | A |
| ATOM | 307 | CB | HIS | A | 138 | 27.675 | 25.634 | 7.864 | 1.00 | 9.77 | A |
| ATOM | 308 | CG | HIS | A | 138 | 26.672 | 26.585 | 7.280 | 1.00 | 9.79 | A |
| ATOM | 309 | CD2 | HIS | A | 138 | 25.904 | 27.537 | 7.861 | 1.00 | 10.42 | A |
| ATOM | 310 | ND1 | HIS | A | 138 | 26.385 | 26.629 | 5.933 | 1.00 | 10.42 | A |
| ATOM | 311 | CE1 | HIS | A | 138 | 25.482 | 27.570 | 5.708 | 1.00 | 12.62 | A |
| ATOM | 312 | NE2 | HIS | A | 138 | 25.175 | 28.136 | 6.860 | 1.00 | 10.74 | A |
| ATOM | 313 | C | HIS | A | 138 | 30.070 | 25.384 | 8.549 | 1.00 | 8.06 | A |
| ATOM | 314 | O | HIS | A | 138 | 30.481 | 26.091 | 9.465 | 1.00 | 9.19 | A |
| ATOM | 315 | N | THR | A | 139 | 30.412 | 24.107 | 8.422 | 1.00 | 7.84 | A |
| ATOM | 316 | CA | THR | A | 139 | 31.306 | 23.489 | 9.395 | 1.00 | 8.21 | A |
| ATOM | 317 | CB | THR | A | 139 | 31.439 | 21.970 | 9.154 | 1.00 | 9.18 | A |
| ATOM | 318 | OG1 | THR | A | 139 | 30.147 | 21.358 | 9.273 | 1.00 | 11.07 | A |
| ATOM | 319 | CG2 | THR | A | 139 | 32.372 | 21.344 | 10.186 | 1.00 | 9.48 | A |
| ATOM | 320 | C | THR | A | 139 | 32.684 | 24.151 | 9.336 | 1.00 | 8.27 | A |
| ATOM | 321 | O | THR | A | 139 | 33.249 | 24.504 | 10.365 | 1.00 | 8.65 | A |
| ATOM | 322 | N | LEU | A | 140 | 33.208 | 24.328 | 8.126 | 1.00 | 6.73 | A |
| ATOM | 323 | CA | LEU | A | 140 | 34.516 | 24.952 | 7.936 | 1.00 | 7.10 | A |
| ATOM | 324 | CB | LEU | A | 140 | 34.900 | 24.938 | 6.454 | 1.00 | 6.22 | A |
| ATOM | 325 | CG | LEU | A | 140 | 35.191 | 23.585 | 5.806 | 1.00 | 7.89 | A |
| ATOM | 326 | CD1 | LEU | A | 140 | 35.368 | 23.765 | 4.298 | 1.00 | 9.36 | A |
| ATOM | 327 | CD2 | LEU | A | 140 | 36.446 | 22.975 | 6.425 | 1.00 | 10.17 | A |
| ATOM | 328 | C | LEU | A | 140 | 34.572 | 26.389 | 8.447 | 1.00 | 8.54 | A |
| ATOM | 329 | O | LEU | A | 140 | 35.629 | 26.856 | 8.879 | 1.00 | 8.74 | A |
| ATOM | 330 | N | ALA | A | 141 | 33.444 | 27.094 | 8.380 | 1.00 | 8.10 | A |
| ATOM | 331 | CA | ALA | A | 141 | 33.397 | 28.479 | 8.840 | 1.00 | 7.81 | A |
| ATOM | 332 | CB | ALA | A | 141 | 32.044 | 29.098 | 8.513 | 1.00 | 7.95 | A |
| ATOM | 333 | C | ALA | A | 141 | 33.664 | 28.551 | 10.339 | 1.00 | 8.11 | A |
| ATOM | 334 | O | ALA | A | 141 | 34.018 | 29.612 | 10.871 | 1.00 | 8.73 | A |
| ATOM | 335 | N | VAL | A | 142 | 33.488 | 27.419 | 11.018 | 1.00 | 7.57 | A |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 336 | CA | VAL | A | 142 | 33.746 | 27.349 | 12.450 | 1.00 | 8.68 | A |
| ATOM | 337 | CB | VAL | A | 142 | 32.628 | 26.579 | 13.187 | 1.00 | 8.53 | A |
| ATOM | 338 | CG1 | VAL | A | 142 | 32.926 | 26.526 | 14.693 | 1.00 | 9.23 | A |
| ATOM | 339 | CG2 | VAL | A | 142 | 31.292 | 27.270 | 12.946 | 1.00 | 9.18 | A |
| ATOM | 340 | C | VAL | A | 142 | 35.087 | 26.674 | 12.742 | 1.00 | 8.97 | A |
| ATOM | 341 | O | VAL | A | 142 | 35.889 | 27.197 | 13.517 | 1.00 | 10.90 | A |
| ATOM | 342 | N | THR | A | 143 | 35.345 | 25.525 | 12.121 | 1.00 | 9.37 | A |
| ATOM | 343 | CA | THR | A | 143 | 36.601 | 24.819 | 12.378 | 1.00 | 9.23 | A |
| ATOM | 344 | CB | THR | A | 143 | 36.637 | 23.422 | 11.716 | 1.00 | 9.23 | A |
| ATOM | 345 | OG1 | THR | A | 143 | 36.497 | 23.550 | 10.295 | 1.00 | 9.23 | A |
| ATOM | 346 | CG2 | THR | A | 143 | 35.521 | 22.546 | 12.274 | 1.00 | 9.22 | A |
| ATOM | 347 | C | THR | A | 143 | 37.839 | 25.591 | 11.945 | 1.00 | 9.03 | A |
| ATOM | 348 | O | THR | A | 143 | 38.929 | 25.348 | 12.456 | 1.00 | 10.11 | A |
| ATOM | 349 | N | CYS | A | 144 | 37.688 | 26.522 | 11.010 | 1.00 | 8.10 | A |
| ATOM | 350 | CA | CYS | A | 144 | 38.848 | 27.294 | 10.580 | 1.00 | 9.39 | A |
| ATOM | 351 | CB | CYS | A | 144 | 38.514 | 28.139 | 9.345 | 1.00 | 9.38 | A |
| ATOM | 352 | SG | CYS | A | 144 | 37.374 | 29.498 | 9.667 | 1.00 | 12.00 | A |
| ATOM | 353 | C | CYS | A | 144 | 39.315 | 28.200 | 11.719 | 1.00 | 9.07 | A |
| ATOM | 354 | O | CYS | A | 144 | 40.447 | 28.680 | 11.712 | 1.00 | 10.50 | A |
| ATOM | 355 | N | GLN | A | 145 | 38.447 | 28.403 | 12.709 | 1.00 | 8.72 | A |
| ATOM | 356 | CA | GLN | A | 145 | 38.755 | 29.256 | 13.858 | 1.00 | 10.01 | A |
| ATOM | 357 | CB | GLN | A | 145 | 37.465 | 29.865 | 14.403 | 1.00 | 10.49 | A |
| ATOM | 358 | CG | GLN | A | 145 | 36.725 | 30.720 | 13.387 | 1.00 | 11.33 | A |
| ATOM | 359 | CD | GLN | A | 145 | 35.499 | 31.375 | 13.976 | 1.00 | 13.67 | A |
| ATOM | 360 | OE1 | GLN | A | 145 | 35.543 | 31.907 | 15.086 | 1.00 | 14.78 | A |
| ATOM | 361 | NE2 | GLN | A | 145 | 34.398 | 31.355 | 13.234 | 1.00 | 10.01 | A |
| ATOM | 362 | C | GLN | A | 145 | 39.477 | 28.521 | 14.985 | 1.00 | 10.04 | A |
| ATOM | 363 | O | GLN | A | 145 | 39.982 | 29.143 | 15.926 | 1.00 | 11.00 | A |
| ATOM | 364 | N | LEU | A | 146 | 39.524 | 27.198 | 14.886 | 1.00 | 9.00 | A |
| ATOM | 365 | CA | LEU | A | 146 | 40.179 | 26.373 | 15.898 | 1.00 | 10.62 | A |
| ATOM | 366 | CB | LEU | A | 146 | 39.875 | 24.893 | 15.653 | 1.00 | 10.21 | A |
| ATOM | 367 | CG | LEU | A | 146 | 38.469 | 24.337 | 15.874 | 1.00 | 11.36 | A |
| ATOM | 368 | CD1 | LEU | A | 146 | 38.393 | 22.952 | 15.256 | 1.00 | 11.83 | A |
| ATOM | 369 | CD2 | LEU | A | 146 | 38.151 | 24.280 | 17.365 | 1.00 | 15.14 | A |
| ATOM | 370 | C | LEU | A | 146 | 41.692 | 26.528 | 15.932 | 1.00 | 11.26 | A |
| ATOM | 371 | O | LEU | A | 146 | 42.309 | 26.979 | 14.968 | 1.00 | 11.50 | A |
| ATOM | 372 | N | PRO | A | 147 | 42.309 | 26.178 | 17.070 | 1.00 | 12.58 | A |
| ATOM | 373 | CD | PRO | A | 147 | 41.680 | 25.866 | 18.367 | 1.00 | 12.30 | A |
| ATOM | 374 | CA | PRO | A | 147 | 43.764 | 26.265 | 17.202 | 1.00 | 11.87 | A |
| ATOM | 375 | CB | PRO | A | 147 | 44.010 | 25.732 | 18.608 | 1.00 | 13.51 | A |
| ATOM | 376 | CG | PRO | A | 147 | 42.792 | 26.180 | 19.349 | 1.00 | 13.16 | A |
| ATOM | 377 | C | PRO | A | 147 | 44.320 | 25.316 | 16.139 | 1.00 | 11.90 | A |
| ATOM | 378 | O | PRO | A | 147 | 43.670 | 24.321 | 15.796 | 1.00 | 12.36 | A |
| ATOM | 379 | N | ILE | A | 148 | 45.505 | 25.602 | 15.620 | 1.00 | 12.68 | A |
| ATOM | 380 | CA | ILE | A | 148 | 46.072 | 24.736 | 14.596 | 1.00 | 13.79 | A |
| ATOM | 381 | CB | ILE | A | 148 | 47.433 | 25.279 | 14.105 | 1.00 | 15.52 | A |
| ATOM | 382 | CG2 | ILE | A | 148 | 48.074 | 24.290 | 13.141 | 1.00 | 16.43 | A |
| ATOM | 383 | CG1 | ILE | A | 148 | 47.216 | 26.625 | 13.397 | 1.00 | 19.02 | A |
| ATOM | 384 | CD1 | ILE | A | 148 | 48.492 | 27.326 | 12.980 | 1.00 | 23.77 | A |
| ATOM | 385 | C | ILE | A | 148 | 46.212 | 23.285 | 15.060 | 1.00 | 12.90 | A |
| ATOM | 386 | O | ILE | A | 148 | 45.996 | 22.361 | 14.277 | 1.00 | 12.36 | A |
| ATOM | 387 | N | ASP | A | 149 | 46.538 | 23.074 | 16.335 | 1.00 | 13.06 | A |
| ATOM | 388 | CA | ASP | A | 149 | 46.687 | 21.708 | 16.833 | 1.00 | 13.17 | A |
| ATOM | 389 | CB | ASP | A | 149 | 47.367 | 21.698 | 18.213 | 1.00 | 14.99 | A |
| ATOM | 390 | CG | ASP | A | 149 | 46.454 | 22.178 | 19.326 | 1.00 | 15.68 | A |
| ATOM | 391 | OD1 | ASP | A | 149 | 46.334 | 23.404 | 19.522 | 1.00 | 15.33 | A |
| ATOM | 392 | OD2 | ASP | A | 149 | 45.856 | 21.318 | 20.005 | 1.00 | 18.19 | A |
| ATOM | 393 | C | ASP | A | 149 | 45.368 | 20.926 | 16.894 | 1.00 | 14.26 | A |
| ATOM | 394 | O | ASP | A | 149 | 45.374 | 19.700 | 17.034 | 1.00 | 14.29 | A |
| ATOM | 395 | N | ARG | A | 150 | 44.237 | 21.624 | 16.789 | 1.00 | 11.56 | A |
| ATOM | 396 | CA | ARG | A | 150 | 42.940 | 20.954 | 16.810 | 1.00 | 12.66 | A |
| ATOM | 397 | CB | ARG | A | 150 | 41.936 | 21.724 | 17.676 | 1.00 | 13.00 | A |
| ATOM | 398 | CG | ARG | A | 150 | 42.306 | 21.817 | 19.157 | 1.00 | 13.36 | A |
| ATOM | 399 | CD | ARG | A | 150 | 41.143 | 22.378 | 19.964 | 1.00 | 12.59 | A |
| ATOM | 400 | NE | ARG | A | 150 | 40.019 | 21.444 | 19.975 | 1.00 | 12.66 | A |
| ATOM | 401 | CZ | ARG | A | 150 | 38.785 | 21.745 | 20.369 | 1.00 | 13.24 | A |
| ATOM | 402 | NH1 | ARG | A | 150 | 38.494 | 22.967 | 20.791 | 1.00 | 13.27 | A |
| ATOM | 403 | NH2 | ARG | A | 150 | 37.838 | 20.815 | 20.338 | 1.00 | 13.59 | A |

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ATOM    404  C   ARG A 150      42.391  20.819  15.390  1.00 13.09      A
ATOM    405  O   ARG A 150      41.246  20.404  15.195  1.00 13.09      A
ATOM    406  N   GLY A 151      43.212  21.183  14.407  1.00 12.45      A
ATOM    407  CA  GLY A 151      42.797  21.082  13.017  1.00 12.19      A
ATOM    408  C   GLY A 151      42.254  22.366  12.423  1.00 11.65      A
ATOM    409  O   GLY A 151      41.647  22.354  11.353  1.00 12.49      A
ATOM    410  N   GLY A 152      42.472  23.484  13.106  1.00 11.30      A
ATOM    411  CA  GLY A 152      41.969  24.747  12.599  1.00 10.67      A
ATOM    412  C   GLY A 152      43.004  25.589  11.885  1.00 11.78      A
ATOM    413  O   GLY A 152      44.135  25.155  11.659  1.00 10.04      A
ATOM    414  N   GLY A 153      42.603  26.805  11.522  1.00 11.68      A
ATOM    415  CA  GLY A 153      43.504  27.713  10.842  1.00 12.29      A
ATOM    416  C   GLY A 153      43.735  28.967  11.661  1.00 11.95      A
ATOM    417  O   GLY A 153      44.413  29.892  11.210  1.00 14.26      A
ATOM    418  N   GLU A 154      43.178  28.991  12.870  1.00 13.09      A
ATOM    419  CA  GLU A 154      43.310  30.138  13.765  1.00 13.65      A
ATOM    420  CB  GLU A 154      44.722  30.185  14.359  1.00 15.09      A
ATOM    421  CG  GLU A 154      44.924  29.184  15.479  1.00 17.51      A
ATOM    422  CD  GLU A 154      46.372  29.050  15.907  1.00 21.30      A
ATOM    423  OE1 GLU A 154      47.095  30.070  15.921  1.00 21.05      A
ATOM    424  OE2 GLU A 154      46.779  27.920  16.244  1.00 21.68      A
ATOM    425  C   GLU A 154      43.000  31.447  13.045  1.00 13.66      A
ATOM    426  O   GLU A 154      43.714  32.439  13.193  1.00 15.59      A
ATOM    427  N   GLY A 155      41.921  31.444  12.271  1.00 12.01      A
ATOM    428  CA  GLY A 155      41.549  32.638  11.540  1.00 11.09      A
ATOM    429  C   GLY A 155      40.055  32.792  11.354  1.00 11.53      A
ATOM    430  O   GLY A 155      39.278  31.872  11.616  1.00 10.72      A
ATOM    431  N   LYS A 156      39.654  33.976  10.903  1.00 11.50      A
ATOM    432  CA  LYS A 156      38.252  34.277  10.655  1.00 11.09      A
ATOM    433  CB  LYS A 156      38.048  35.789  10.561  1.00 11.40      A
ATOM    434  CG  LYS A 156      38.265  36.533  11.863  1.00 14.73      A
ATOM    435  CD  LYS A 156      38.168  38.031  11.616  1.00 18.50      A
ATOM    436  CE  LYS A 156      38.158  38.814  12.916  1.00 21.90      A
ATOM    437  NZ  LYS A 156      38.016  40.271  12.640  1.00 26.01      A
ATOM    438  C   LYS A 156      37.789  33.643   9.352  1.00 10.36      A
ATOM    439  O   LYS A 156      38.599  33.213   8.529  1.00  9.77      A
ATOM    440  N   ALA A 157      36.477  33.593   9.168  1.00  9.56      A
ATOM    441  CA  ALA A 157      35.919  33.037   7.949  1.00  8.82      A
ATOM    442  CB  ALA A 157      35.042  31.831   8.262  1.00  9.17      A
ATOM    443  C   ALA A 157      35.093  34.085   7.234  1.00 10.33      A
ATOM    444  O   ALA A 157      34.468  34.942   7.860  1.00 10.06      A
ATOM    445  N   MSE   158      35.099  34.006   5.912   .54  9.17      AC1
ATOM    446  CA  MSE   158      34.321  34.913   5.097   .54 10.42      AC1
ATOM    447  CB  MSE   158      35.231  35.701   4.174   .54 11.72      AC1
ATOM    448  CG  MSE   158      34.551  36.879   3.548   .54 13.13      AC1
ATOM    449  SE  MSE   158      35.839  37.882   2.572   .54 15.92      AC1
ATOM    450  CE  MSE   158      37.003  38.379   4.022   .54 11.46      AC1
ATOM    451  C   MSE   158      33.391  34.013   4.298   .54 10.25      AC1
ATOM    452  O   MSE   158      33.830  33.034   3.694   .54 10.22      AC1
ATOM    453  N   TYR A 159      32.106  34.343   4.304  1.00 10.25      A
ATOM    454  CA  TYR A 159      31.111  33.534   3.616  1.00 10.01      A
ATOM    455  CB  TYR A 159      30.201  32.892   4.676  1.00  9.57      A
ATOM    456  CG  TYR A 159      29.410  31.677   4.242  1.00 10.37      A
ATOM    457  CD1 TYR A 159      28.533  31.730   3.158  1.00 11.98      A
ATOM    458  CE1 TYR A 159      27.786  30.609   2.783  1.00 13.38      A
ATOM    459  CD2 TYR A 159      29.520  30.474   4.943  1.00 11.85      A
ATOM    460  CE2 TYR A 159      28.777  29.350   4.576  1.00 11.39      A
ATOM    461  CZ  TYR A 159      27.914  29.425   3.498  1.00 13.64      A
ATOM    462  OH  TYR A 159      27.187  28.315   3.136  1.00 14.59      A
ATOM    463  C   TYR A 159      30.267  34.333   2.630  1.00 10.25      A
ATOM    464  O   TYR A 159      29.432  35.139   3.038  1.00 10.49      A
ATOM    465  N   ILE A 160      30.490  34.115   1.336  1.00  9.28      A
ATOM    466  CA  ILE A 160      29.705  34.792    .314  1.00  9.69      A
ATOM    467  CB  ILE A 160      30.568  35.214   -.896  1.00  9.03      A
ATOM    468  CG2 ILE A 160      29.678  35.780  -1.999  1.00 13.08      A
ATOM    469  CG1 ILE A 160      31.592  36.265   -.458  1.00 10.09      A
ATOM    470  CD1 ILE A 160      32.556  36.699  -1.554  1.00  8.81      A
ATOM    471  C   ILE A 160      28.645  33.794   -.135  1.00 10.60      A
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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 472 | O | ILE | A | 160 | 28.960 | 32.751 | -.708 | 1.00 | 10.08 | A |
| ATOM | 473 | N | ASP | A | 161 | 27.390 | 34.117 | .155 | 1.00 | 11.32 | A |
| ATOM | 474 | CA | ASP | A | 161 | 26.263 | 33.260 | -.192 | 1.00 | 12.57 | A |
| ATOM | 475 | CB | ASP | A | 161 | 25.293 | 33.175 | .994 | 1.00 | 13.81 | A |
| ATOM | 476 | CG | ASP | A | 161 | 23.963 | 32.540 | .619 | 1.00 | 16.41 | A |
| ATOM | 477 | OD1 | ASP | A | 161 | 23.936 | 31.323 | .345 | 1.00 | 17.20 | A |
| ATOM | 478 | OD2 | ASP | A | 161 | 22.945 | 33.267 | .589 | 1.00 | 19.96 | A |
| ATOM | 479 | C | ASP | A | 161 | 25.520 | 33.815 | -1.399 | 1.00 | 13.45 | A |
| ATOM | 480 | O | ASP | A | 161 | 25.437 | 35.027 | -1.577 | 1.00 | 15.58 | A |
| ATOM | 481 | N | THR | A | 162 | 24.984 | 32.925 | -2.226 | 1.00 | 15.93 | A |
| ATOM | 482 | CA | THR | A | 162 | 24.221 | 33.347 | -3.396 | 1.00 | 16.70 | A |
| ATOM | 483 | CB | THR | A | 162 | 24.949 | 33.011 | -4.718 | 1.00 | 16.70 | A |
| ATOM | 484 | OG1 | THR | A | 162 | 24.979 | 31.588 | -4.897 | 1.00 | 17.06 | A |
| ATOM | 485 | CG2 | THR | A | 162 | 26.371 | 33.555 | -4.708 | 1.00 | 16.05 | A |
| ATOM | 486 | C | THR | A | 162 | 22.898 | 32.594 | -3.409 | 1.00 | 18.68 | A |
| ATOM | 487 | O | THR | A | 162 | 22.012 | 32.894 | -4.212 | 1.00 | 19.52 | A |
| ATOM | 488 | N | GLU | A | 163 | 22.771 | 31.629 | -2.501 | 1.00 | 18.38 | A |
| ATOM | 489 | CA | GLU | A | 163 | 21.589 | 30.772 | -2.425 | 1.00 | 20.29 | A |
| ATOM | 490 | CB | GLU | A | 163 | 22.031 | 29.318 | -2.260 | 1.00 | 20.64 | A |
| ATOM | 491 | CG | GLU | A | 163 | 23.048 | 28.837 | -3.278 | 1.00 | 25.07 | A |
| ATOM | 492 | CD | GLU | A | 163 | 22.527 | 28.909 | -4.696 | 1.00 | 27.45 | A |
| ATOM | 493 | OE1 | GLU | A | 163 | 22.624 | 29.991 | -5.315 | 1.00 | 26.80 | A |
| ATOM | 494 | OE2 | GLU | A | 163 | 22.009 | 27.883 | -5.184 | 1.00 | 28.60 | A |
| ATOM | 495 | C | GLU | A | 163 | 20.573 | 31.078 | -1.332 | 1.00 | 20.03 | A |
| ATOM | 496 | O | GLU | A | 163 | 19.466 | 30.539 | -1.354 | 1.00 | 21.59 | A |
| ATOM | 497 | N | GLY | A | 164 | 20.948 | 31.915 | -.372 | 1.00 | 19.41 | A |
| ATOM | 498 | CA | GLY | A | 164 | 20.043 | 32.234 | .718 | 1.00 | 19.90 | A |
| ATOM | 499 | C | GLY | A | 164 | 19.981 | 31.097 | 1.723 | 1.00 | 19.77 | A |
| ATOM | 500 | O | GLY | A | 164 | 18.979 | 30.919 | 2.419 | 1.00 | 19.85 | A |
| ATOM | 501 | N | THR | A | 165 | 21.059 | 30.323 | 1.807 | 1.00 | 15.75 | A |
| ATOM | 502 | CA | THR | A | 165 | 21.106 | 29.193 | 2.729 | 1.00 | 16.97 | A |
| ATOM | 503 | CB | THR | A | 165 | 21.388 | 27.879 | 1.973 | 1.00 | 16.58 | A |
| ATOM | 504 | OG1 | THR | A | 165 | 22.474 | 28.074 | 1.057 | 1.00 | 16.41 | A |
| ATOM | 505 | CG2 | THR | A | 165 | 20.149 | 27.435 | 1.205 | 1.00 | 19.06 | A |
| ATOM | 506 | C | THR | A | 165 | 22.117 | 29.344 | 3.864 | 1.00 | 16.78 | A |
| ATOM | 507 | O | THR | A | 165 | 22.512 | 28.359 | 4.492 | 1.00 | 16.85 | A |
| ATOM | 508 | N | PHE | A | 166 | 22.543 | 30.574 | 4.125 | 1.00 | 15.79 | A |
| ATOM | 509 | CA | PHE | A | 166 | 23.477 | 30.820 | 5.217 | 1.00 | 14.36 | A |
| ATOM | 510 | CB | PHE | A | 166 | 24.153 | 32.181 | 5.058 | 1.00 | 13.90 | A |
| ATOM | 511 | CG | PHE | A | 166 | 25.137 | 32.498 | 6.154 | 1.00 | 13.95 | A |
| ATOM | 512 | CD1 | PHE | A | 166 | 26.357 | 31.829 | 6.230 | 1.00 | 13.42 | A |
| ATOM | 513 | CD2 | PHE | A | 166 | 24.840 | 33.462 | 7.115 | 1.00 | 13.77 | A |
| ATOM | 514 | CE1 | PHE | A | 166 | 27.270 | 32.119 | 7.248 | 1.00 | 13.37 | A |
| ATOM | 515 | CE2 | PHE | A | 166 | 25.744 | 33.759 | 8.135 | 1.00 | 13.84 | A |
| ATOM | 516 | CZ | PHE | A | 166 | 26.963 | 33.086 | 8.202 | 1.00 | 14.21 | A |
| ATOM | 517 | C | PHE | A | 166 | 22.650 | 30.805 | 6.498 | 1.00 | 16.02 | A |
| ATOM | 518 | O | PHE | A | 166 | 21.637 | 31.502 | 6.592 | 1.00 | 15.82 | A |
| ATOM | 519 | N | ARG | A | 167 | 23.073 | 30.018 | 7.482 | 1.00 | 14.61 | A |
| ATOM | 520 | CA | ARG | A | 167 | 22.333 | 29.919 | 8.738 | 1.00 | 15.67 | A |
| ATOM | 521 | CB | ARG | A | 167 | 21.574 | 28.590 | 8.785 | 1.00 | 17.46 | A |
| ATOM | 522 | CG | ARG | A | 167 | 20.523 | 28.425 | 7.695 | 1.00 | 21.67 | A |
| ATOM | 523 | CD | ARG | A | 167 | 19.307 | 29.307 | 7.944 | 1.00 | 26.33 | A |
| ATOM | 524 | NE | ARG | A | 167 | 18.267 | 29.086 | 6.940 | 1.00 | 30.64 | A |
| ATOM | 525 | CZ | ARG | A | 167 | 18.256 | 29.639 | 5.731 | 1.00 | 32.90 | A |
| ATOM | 526 | NH1 | ARG | A | 167 | 19.229 | 30.462 | 5.362 | 1.00 | 32.52 | A |
| ATOM | 527 | NH2 | ARG | A | 167 | 17.272 | 29.362 | 4.884 | 1.00 | 34.53 | A |
| ATOM | 528 | C | ARG | A | 167 | 23.206 | 30.046 | 9.984 | 1.00 | 14.69 | A |
| ATOM | 529 | O | ARG | A | 167 | 23.897 | 29.099 | 10.375 | 1.00 | 13.43 | A |
| ATOM | 530 | N | PRO | A | 168 | 23.186 | 31.223 | 10.627 | 1.00 | 14.89 | A |
| ATOM | 531 | CD | PRO | A | 168 | 22.557 | 32.476 | 10.172 | 1.00 | 14.33 | A |
| ATOM | 532 | CA | PRO | A | 168 | 23.984 | 31.445 | 11.836 | 1.00 | 15.39 | A |
| ATOM | 533 | CB | PRO | A | 168 | 23.561 | 32.846 | 12.273 | 1.00 | 14.97 | A |
| ATOM | 534 | CG | PRO | A | 168 | 23.315 | 33.530 | 10.956 | 1.00 | 15.63 | A |
| ATOM | 535 | C | PRO | A | 168 | 23.738 | 30.391 | 12.919 | 1.00 | 16.84 | A |
| ATOM | 536 | O | PRO | A | 168 | 24.656 | 30.028 | 13.654 | 1.00 | 16.46 | A |
| ATOM | 537 | N | GLU | A | 169 | 22.508 | 29.887 | 13.015 | 1.00 | 17.31 | A |
| ATOM | 538 | CA | GLU | A | 169 | 22.208 | 28.886 | 14.036 | 1.00 | 18.18 | A |
| ATOM | 539 | CB | GLU | A | 169 | 20.714 | 28.538 | 14.055 | 1.00 | 21.53 | A |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 540 | CG | GLU | A | 169 | 20.140 | 28.117 | 12.717 | 1.00 | 26.55 | A |
| ATOM | 541 | CD | GLU | A | 169 | 19.394 | 29.242 | 12.019 | 1.00 | 30.20 | A |
| ATOM | 542 | OE1 | GLU | A | 169 | 19.999 | 30.309 | 11.762 | 1.00 | 27.11 | A |
| ATOM | 543 | OE2 | GLU | A | 169 | 18.194 | 29.050 | 11.728 | 1.00 | 32.63 | A |
| ATOM | 544 | C | GLU | A | 169 | 23.029 | 27.614 | 13.861 | 1.00 | 16.74 | A |
| ATOM | 545 | O | GLU | A | 169 | 23.365 | 26.949 | 14.844 | 1.00 | 15.48 | A |
| ATOM | 546 | N | ARG | A | 170 | 23.349 | 27.268 | 12.615 | 1.00 | 14.29 | A |
| ATOM | 547 | CA | ARG | A | 170 | 24.149 | 26.077 | 12.363 | 1.00 | 13.93 | A |
| ATOM | 548 | CB | ARG | A | 170 | 24.206 | 25.757 | 10.867 | 1.00 | 15.66 | A |
| ATOM | 549 | CG | ARG | A | 170 | 25.057 | 24.536 | 10.535 | 1.00 | 20.09 | A |
| ATOM | 550 | CD | ARG | A | 170 | 24.452 | 23.251 | 11.095 | 1.00 | 23.76 | A |
| ATOM | 551 | NE | ARG | A | 170 | 23.147 | 22.970 | 10.502 | 1.00 | 28.96 | A |
| ATOM | 552 | CZ | ARG | A | 170 | 22.019 | 22.859 | 11.197 | 1.00 | 31.03 | A |
| ATOM | 553 | NH1 | ARG | A | 170 | 22.031 | 23.000 | 12.514 | 1.00 | 33.04 | A |
| ATOM | 554 | NH2 | ARG | A | 170 | 20.875 | 22.616 | 10.573 | 1.00 | 35.19 | A |
| ATOM | 555 | C | ARG | A | 170 | 25.557 | 26.301 | 12.899 | 1.00 | 13.95 | A |
| ATOM | 556 | O | ARG | A | 170 | 26.167 | 25.387 | 13.455 | 1.00 | 12.96 | A |
| ATOM | 557 | N | LEU | A | 171 | 26.070 | 27.518 | 12.736 | 1.00 | 12.17 | A |
| ATOM | 558 | CA | LEU | A | 171 | 27.407 | 27.839 | 13.233 | 1.00 | 11.76 | A |
| ATOM | 559 | CB | LEU | A | 171 | 27.796 | 29.269 | 12.854 | 1.00 | 12.30 | A |
| ATOM | 560 | CG | LEU | A | 171 | 27.693 | 29.625 | 11.371 | 1.00 | 11.31 | A |
| ATOM | 561 | CD1 | LEU | A | 171 | 28.133 | 31.070 | 11.170 | 1.00 | 12.66 | A |
| ATOM | 562 | CD2 | LEU | A | 171 | 28.552 | 28.677 | 10.546 | 1.00 | 12.20 | A |
| ATOM | 563 | C | LEU | A | 171 | 27.447 | 27.687 | 14.755 | 1.00 | 11.70 | A |
| ATOM | 564 | O | LEU | A | 171 | 28.425 | 27.190 | 15.311 | 1.00 | 11.76 | A |
| ATOM | 565 | N | LEU | A | 172 | 26.382 | 28.114 | 15.427 | 1.00 | 11.75 | A |
| ATOM | 566 | CA | LEU | A | 172 | 26.321 | 28.001 | 16.880 | 1.00 | 12.10 | A |
| ATOM | 567 | CB | LEU | A | 172 | 25.049 | 28.656 | 17.424 | 1.00 | 12.80 | A |
| ATOM | 568 | CG | LEU | A | 172 | 24.981 | 30.178 | 17.302 | 1.00 | 14.86 | A |
| ATOM | 569 | CD1 | LEU | A | 172 | 23.659 | 30.671 | 17.874 | 1.00 | 16.13 | A |
| ATOM | 570 | CD2 | LEU | A | 172 | 26.153 | 30.811 | 18.043 | 1.00 | 15.33 | A |
| ATOM | 571 | C | LEU | A | 172 | 26.379 | 26.546 | 17.324 | 1.00 | 12.23 | A |
| ATOM | 572 | O | LEU | A | 172 | 27.018 | 26.227 | 18.326 | 1.00 | 12.62 | A |
| ATOM | 573 | N | ALA | A | 173 | 25.712 | 25.665 | 16.580 | 1.00 | 12.72 | A |
| ATOM | 574 | CA | ALA | A | 173 | 25.713 | 24.245 | 16.919 | 1.00 | 13.14 | A |
| ATOM | 575 | CB | ALA | A | 173 | 24.720 | 23.486 | 16.041 | 1.00 | 11.87 | A |
| ATOM | 576 | C | ALA | A | 173 | 27.112 | 23.665 | 16.747 | 1.00 | 12.63 | A |
| ATOM | 577 | O | ALA | A | 173 | 27.578 | 22.894 | 17.581 | 1.00 | 11.33 | A |
| ATOM | 578 | N | VAL | A | 174 | 27.787 | 24.034 | 15.662 | 1.00 | 10.42 | A |
| ATOM | 579 | CA | VAL | A | 174 | 29.133 | 23.534 | 15.428 | 1.00 | 9.27 | A |
| ATOM | 580 | CB | VAL | A | 174 | 29.662 | 23.953 | 14.041 | 1.00 | 9.04 | A |
| ATOM | 581 | CG1 | VAL | A | 174 | 31.093 | 23.458 | 13.861 | 1.00 | 8.42 | A |
| ATOM | 582 | CG2 | VAL | A | 174 | 28.763 | 23.386 | 12.955 | 1.00 | 9.09 | A |
| ATOM | 583 | C | VAL | A | 174 | 30.075 | 24.073 | 16.499 | 1.00 | 10.17 | A |
| ATOM | 584 | O | VAL | A | 174 | 30.953 | 23.358 | 16.977 | 1.00 | 10.23 | A |
| ATOM | 585 | N | ALA | A | 175 | 29.886 | 25.335 | 16.877 | 1.00 | 9.90 | A |
| ATOM | 586 | CA | ALA | A | 175 | 30.725 | 25.951 | 17.897 | 1.00 | 10.67 | A |
| ATOM | 587 | CB | ALA | A | 175 | 30.316 | 27.407 | 18.108 | 1.00 | 11.94 | A |
| ATOM | 588 | C | ALA | A | 175 | 30.611 | 25.182 | 19.208 | 1.00 | 11.92 | A |
| ATOM | 589 | O | ALA | A | 175 | 31.616 | 24.883 | 19.847 | 1.00 | 11.33 | A |
| ATOM | 590 | N | GLU | A | 176 | 29.383 | 24.854 | 19.600 | 1.00 | 13.20 | A |
| ATOM | 591 | CA | GLU | A | 176 | 29.163 | 24.119 | 20.845 | 1.00 | 13.21 | A |
| ATOM | 592 | CB | GLU | A | 176 | 27.664 | 23.932 | 21.099 | 1.00 | 15.61 | A |
| ATOM | 593 | CG | GLU | A | 176 | 27.349 | 23.074 | 22.326 | 1.00 | 19.61 | A |
| ATOM | 594 | CD | GLU | A | 176 | 25.879 | 23.099 | 22.705 | 1.00 | 23.95 | A |
| ATOM | 595 | OE1 | GLU | A | 176 | 25.027 | 23.172 | 21.795 | 1.00 | 25.62 | A |
| ATOM | 596 | OE2 | GLU | A | 176 | 25.573 | 23.030 | 23.916 | 1.00 | 27.39 | A |
| ATOM | 597 | C | GLU | A | 176 | 29.854 | 22.762 | 20.793 | 1.00 | 12.78 | A |
| ATOM | 598 | O | GLU | A | 176 | 30.477 | 22.325 | 21.762 | 1.00 | 13.68 | A |
| ATOM | 599 | N | ARG | A | 177 | 29.740 | 22.099 | 19.650 | 1.00 | 11.89 | A |
| ATOM | 600 | CA | ARG | A | 177 | 30.360 | 20.798 | 19.454 | 1.00 | 11.86 | A |
| ATOM | 601 | CB | ARG | A | 177 | 30.078 | 20.329 | 18.026 | 1.00 | 10.78 | A |
| ATOM | 602 | CG | ARG | A | 177 | 30.928 | 19.176 | 17.542 | 1.00 | 11.79 | A |
| ATOM | 603 | CD | ARG | A | 177 | 30.643 | 18.947 | 16.070 | 1.00 | 12.75 | A |
| ATOM | 604 | NE | ARG | A | 177 | 31.478 | 17.900 | 15.497 | 1.00 | 14.37 | A |
| ATOM | 605 | CZ | ARG | A | 177 | 31.587 | 17.681 | 14.193 | 1.00 | 13.51 | A |
| ATOM | 606 | NH1 | ARG | A | 177 | 30.915 | 18.440 | 13.337 | 1.00 | 13.86 | A |
| ATOM | 607 | NH2 | ARG | A | 177 | 32.366 | 16.708 | 13.746 | 1.00 | 13.82 | A |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 608 | C | ARG | A | 177 | 31.869 | 20.852 | 19.701 | 1.00 | 12.81 | A |
| ATOM | 609 | O | ARG | A | 177 | 32.447 | 19.941 | 20.297 | 1.00 | 11.57 | A |
| ATOM | 610 | N | TYR | A | 178 | 32.510 | 21.924 | 19.243 | 1.00 | 12.95 | A |
| ATOM | 611 | CA | TYR | A | 178 | 33.952 | 22.068 | 19.406 | 1.00 | 12.76 | A |
| ATOM | 612 | CB | TYR | A | 178 | 34.540 | 22.714 | 18.146 | 1.00 | 13.24 | A |
| ATOM | 613 | CG | TYR | A | 178 | 34.686 | 21.722 | 17.018 | 1.00 | 12.79 | A |
| ATOM | 614 | CD1 | TYR | A | 178 | 35.763 | 20.834 | 16.987 | 1.00 | 12.88 | A |
| ATOM | 615 | CE1 | TYR | A | 178 | 35.890 | 19.891 | 15.971 | 1.00 | 14.50 | A |
| ATOM | 616 | CD2 | TYR | A | 178 | 33.736 | 21.642 | 16.002 | 1.00 | 12.10 | A |
| ATOM | 617 | CE2 | TYR | A | 178 | 33.853 | 20.700 | 14.980 | 1.00 | 13.48 | A |
| ATOM | 618 | CZ | TYR | A | 178 | 34.933 | 19.831 | 14.972 | 1.00 | 13.02 | A |
| ATOM | 619 | OH | TYR | A | 178 | 35.066 | 18.902 | 13.966 | 1.00 | 16.93 | A |
| ATOM | 620 | C | TYR | A | 178 | 34.387 | 22.826 | 20.657 | 1.00 | 13.57 | A |
| ATOM | 621 | O | TYR | A | 178 | 35.571 | 23.115 | 20.837 | 1.00 | 14.22 | A |
| ATOM | 622 | N | GLY | A | 179 | 33.427 | 23.140 | 21.522 | 1.00 | 14.01 | A |
| ATOM | 623 | CA | GLY | A | 179 | 33.742 | 23.841 | 22.755 | 1.00 | 14.86 | A |
| ATOM | 624 | C | GLY | A | 179 | 34.238 | 25.260 | 22.561 | 1.00 | 15.37 | A |
| ATOM | 625 | O | GLY | A | 179 | 35.016 | 25.769 | 23.368 | 1.00 | 16.81 | A |
| ATOM | 626 | N | LEU | A | 180 | 33.788 | 25.903 | 21.491 | 1.00 | 14.92 | A |
| ATOM | 627 | CA | LEU | A | 180 | 34.182 | 27.276 | 21.208 | 1.00 | 15.19 | A |
| ATOM | 628 | CB | LEU | A | 180 | 34.468 | 27.447 | 19.719 | 1.00 | 16.63 | A |
| ATOM | 629 | CG | LEU | A | 180 | 35.636 | 26.648 | 19.147 | 1.00 | 15.00 | A |
| ATOM | 630 | CD1 | LEU | A | 180 | 35.705 | 26.872 | 17.641 | 1.00 | 17.63 | A |
| ATOM | 631 | CD2 | LEU | A | 180 | 36.931 | 27.079 | 19.815 | 1.00 | 19.25 | A |
| ATOM | 632 | C | LEU | A | 180 | 33.066 | 28.229 | 21.611 | 1.00 | 16.56 | A |
| ATOM | 633 | O | LEU | A | 180 | 31.897 | 27.842 | 21.669 | 1.00 | 17.28 | A |
| ATOM | 634 | N | SER | A | 181 | 33.434 | 29.475 | 21.891 | 1.00 | 16.35 | A |
| ATOM | 635 | CA | SER | A | 181 | 32.463 | 30.497 | 22.261 | 1.00 | 16.39 | A |
| ATOM | 636 | CB | SER | A | 181 | 33.177 | 31.792 | 22.647 | 1.00 | 17.27 | A |
| ATOM | 637 | OG | SER | A | 181 | 32.259 | 32.871 | 22.715 | 1.00 | 18.74 | A |
| ATOM | 638 | C | SER | A | 181 | 31.556 | 30.764 | 21.067 | 1.00 | 16.14 | A |
| ATOM | 639 | O | SER | A | 181 | 32.029 | 31.173 | 20.009 | 1.00 | 15.41 | A |
| ATOM | 640 | N | GLY | A | 182 | 30.258 | 30.534 | 21.240 | 1.00 | 15.64 | A |
| ATOM | 641 | CA | GLY | A | 182 | 29.320 | 30.759 | 20.156 | 1.00 | 14.80 | A |
| ATOM | 642 | C | GLY | A | 182 | 29.312 | 32.209 | 19.708 | 1.00 | 14.74 | A |
| ATOM | 643 | O | GLY | A | 182 | 29.257 | 32.502 | 18.508 | 1.00 | 14.19 | A |
| ATOM | 644 | N | SER | A | 183 | 29.377 | 33.124 | 20.673 | 1.00 | 16.05 | A |
| ATOM | 645 | CA | SER | A | 183 | 29.377 | 34.549 | 20.365 | 1.00 | 17.71 | A |
| ATOM | 646 | CB | SER | A | 183 | 29.274 | 35.374 | 21.654 | 1.00 | 17.19 | A |
| ATOM | 647 | OG | SER | A | 183 | 30.314 | 35.052 | 22.557 | 1.00 | 21.78 | A |
| ATOM | 648 | C | SER | A | 183 | 30.626 | 34.942 | 19.579 | 1.00 | 16.35 | A |
| ATOM | 649 | O | SER | A | 183 | 30.534 | 35.682 | 18.595 | 1.00 | 16.95 | A |
| ATOM | 650 | N | ASP | A | 184 | 31.789 | 34.453 | 20.006 | 1.00 | 15.79 | A |
| ATOM | 651 | CA | ASP | A | 184 | 33.028 | 34.754 | 19.297 | 1.00 | 15.34 | A |
| ATOM | 652 | CB | ASP | A | 184 | 34.243 | 34.153 | 20.009 | 1.00 | 17.96 | A |
| ATOM | 653 | CG | ASP | A | 184 | 34.646 | 34.928 | 21.244 | 1.00 | 21.29 | A |
| ATOM | 654 | OD1 | ASP | A | 184 | 34.198 | 36.082 | 21.401 | 1.00 | 22.54 | A |
| ATOM | 655 | OD2 | ASP | A | 184 | 35.430 | 34.384 | 22.050 | 1.00 | 24.60 | A |
| ATOM | 656 | C | ASP | A | 184 | 32.966 | 34.183 | 17.884 | 1.00 | 14.07 | A |
| ATOM | 657 | O | ASP | A | 184 | 33.351 | 34.847 | 16.923 | 1.00 | 14.53 | A |
| ATOM | 658 | N | VAL | A | 185 | 32.485 | 32.948 | 17.762 | 1.00 | 12.60 | A |
| ATOM | 659 | CA | VAL | A | 185 | 32.393 | 32.309 | 16.451 | 1.00 | 10.90 | A |
| ATOM | 660 | CB | VAL | A | 185 | 31.812 | 30.875 | 16.565 | 1.00 | 10.19 | A |
| ATOM | 661 | CG1 | VAL | A | 185 | 31.437 | 30.336 | 15.178 | 1.00 | 11.57 | A |
| ATOM | 662 | CG2 | VAL | A | 185 | 32.854 | 29.957 | 17.206 | 1.00 | 11.80 | A |
| ATOM | 663 | C | VAL | A | 185 | 31.552 | 33.139 | 15.483 | 1.00 | 10.62 | A |
| ATOM | 664 | O | VAL | A | 185 | 31.947 | 33.347 | 14.336 | 1.00 | 11.96 | A |
| ATOM | 665 | N | LEU | A | 186 | 30.406 | 33.633 | 15.937 | 1.00 | 11.61 | A |
| ATOM | 666 | CA | LEU | A | 186 | 29.568 | 34.441 | 15.056 | 1.00 | 12.75 | A |
| ATOM | 667 | CB | LEU | A | 186 | 28.206 | 34.719 | 15.698 | 1.00 | 13.84 | A |
| ATOM | 668 | CG | LEU | A | 186 | 27.315 | 33.502 | 15.965 | 1.00 | 15.35 | A |
| ATOM | 669 | CD1 | LEU | A | 186 | 25.951 | 33.981 | 16.429 | 1.00 | 17.79 | A |
| ATOM | 670 | CD2 | LEU | A | 186 | 27.170 | 32.663 | 14.709 | 1.00 | 16.34 | A |
| ATOM | 671 | C | LEU | A | 186 | 30.246 | 35.761 | 14.698 | 1.00 | 12.81 | A |
| ATOM | 672 | O | LEU | A | 186 | 30.136 | 36.235 | 13.565 | 1.00 | 13.44 | A |
| ATOM | 673 | N | ASP | A | 187 | 30.938 | 36.362 | 15.659 | 1.00 | 12.21 | A |
| ATOM | 674 | CA | ASP | A | 187 | 31.619 | 37.627 | 15.394 | 1.00 | 14.99 | A |
| ATOM | 675 | CB | ASP | A | 187 | 32.163 | 38.255 | 16.678 | 1.00 | 16.78 | A |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 676 | CG | ASP | A | 187 | 31.074 | 38.721 | 17.619 | 1.00 | 20.35 | A |
| ATOM | 677 | OD1 | ASP | A | 187 | 29.988 | 39.116 | 17.147 | 1.00 | 21.97 | A |
| ATOM | 678 | OD2 | ASP | A | 187 | 31.324 | 38.706 | 18.843 | 1.00 | 25.56 | A |
| ATOM | 679 | C | ASP | A | 187 | 32.791 | 37.436 | 14.440 | 1.00 | 15.26 | A |
| ATOM | 680 | O | ASP | A | 187 | 33.259 | 38.400 | 13.830 | 1.00 | 15.23 | A |
| ATOM | 681 | N | ASN | A | 188 | 33.270 | 36.200 | 14.322 | 1.00 | 13.87 | A |
| ATOM | 682 | CA | ASN | A | 188 | 34.403 | 35.905 | 13.450 | 1.00 | 14.14 | A |
| ATOM | 683 | CB | ASN | A | 188 | 35.368 | 34.942 | 14.135 | 1.00 | 14.82 | A |
| ATOM | 684 | CG | ASN | A | 188 | 36.110 | 35.587 | 15.281 | 1.00 | 18.85 | A |
| ATOM | 685 | OD1 | ASN | A | 188 | 36.520 | 36.744 | 15.195 | 1.00 | 20.12 | A |
| ATOM | 686 | ND2 | ASN | A | 188 | 36.306 | 34.836 | 16.357 | 1.00 | 21.10 | A |
| ATOM | 687 | C | ASN | A | 188 | 34.050 | 35.359 | 12.072 | 1.00 | 13.53 | A |
| ATOM | 688 | O | ASN | A | 188 | 34.929 | 34.904 | 11.343 | 1.00 | 13.36 | A |
| ATOM | 689 | N | VAL | A | 189 | 32.769 | 35.367 | 11.727 | 1.00 | 12.06 | A |
| ATOM | 690 | CA | VAL | A | 189 | 32.357 | 34.924 | 10.402 | 1.00 | 10.87 | A |
| ATOM | 691 | CB | VAL | A | 189 | 31.309 | 33.779 | 10.446 | 1.00 | 9.92 | A |
| ATOM | 692 | CG1 | VAL | A | 189 | 30.851 | 33.443 | 9.026 | 1.00 | 9.91 | A |
| ATOM | 693 | CG2 | VAL | A | 189 | 31.913 | 32.537 | 11.092 | 1.00 | 10.65 | A |
| ATOM | 694 | C | VAL | A | 189 | 31.726 | 36.135 | 9.725 | 1.00 | 13.11 | A |
| ATOM | 695 | O | VAL | A | 189 | 30.705 | 36.642 | 10.187 | 1.00 | 14.95 | A |
| ATOM | 696 | N | ALA | A | 190 | 32.352 | 36.614 | 8.653 | 1.00 | 11.72 | A |
| ATOM | 697 | CA | ALA | A | 190 | 31.825 | 37.753 | 7.905 | 1.00 | 11.20 | A |
| ATOM | 698 | CB | ALA | A | 190 | 32.961 | 38.597 | 7.353 | 1.00 | 10.95 | A |
| ATOM | 699 | C | ALA | A | 190 | 30.992 | 37.170 | 6.773 | 1.00 | 11.60 | A |
| ATOM | 700 | O | ALA | A | 190 | 31.458 | 36.303 | 6.032 | 1.00 | 12.58 | A |
| ATOM | 701 | N | TYR | A | 191 | 29.765 | 37.658 | 6.643 | 1.00 | 9.10 | A |
| ATOM | 702 | CA | TYR | A | 191 | 28.829 | 37.157 | 5.646 | 1.00 | 11.15 | A |
| ATOM | 703 | CB | TYR | A | 191 | 27.653 | 36.493 | 6.377 | 1.00 | 14.31 | A |
| ATOM | 704 | CG | TYR | A | 191 | 26.381 | 36.329 | 5.573 | 1.00 | 16.33 | A |
| ATOM | 705 | CD1 | TYR | A | 191 | 26.292 | 35.384 | 4.550 | 1.00 | 18.03 | A |
| ATOM | 706 | CE1 | TYR | A | 191 | 25.116 | 35.219 | 3.819 | 1.00 | 21.10 | A |
| ATOM | 707 | CD2 | TYR | A | 191 | 25.259 | 37.110 | 5.846 | 1.00 | 19.21 | A |
| ATOM | 708 | CE2 | TYR | A | 191 | 24.077 | 36.955 | 5.120 | 1.00 | 21.77 | A |
| ATOM | 709 | CZ | TYR | A | 191 | 24.012 | 36.007 | 4.110 | 1.00 | 22.07 | A |
| ATOM | 710 | OH | TYR | A | 191 | 22.842 | 35.844 | 3.399 | 1.00 | 24.46 | A |
| ATOM | 711 | C | TYR | A | 191 | 28.296 | 38.219 | 4.701 | 1.00 | 9.98 | A |
| ATOM | 712 | O | TYR | A | 191 | 28.083 | 39.363 | 5.091 | 1.00 | 10.36 | A |
| ATOM | 713 | N | ALA | A | 192 | 28.085 | 37.823 | 3.452 | 1.00 | 9.94 | A |
| ATOM | 714 | CA | ALA | A | 192 | 27.527 | 38.718 | 2.452 | 1.00 | 10.77 | A |
| ATOM | 715 | CB | ALA | A | 192 | 28.635 | 39.455 | 1.709 | 1.00 | 11.74 | A |
| ATOM | 716 | C | ALA | A | 192 | 26.725 | 37.881 | 1.478 | 1.00 | 12.63 | A |
| ATOM | 717 | O | ALA | A | 192 | 27.075 | 36.735 | 1.204 | 1.00 | 13.05 | A |
| ATOM | 718 | N | ARG | A | 193 | 25.630 | 38.432 | .974 | 1.00 | 14.15 | A |
| ATOM | 719 | CA | ARG | A | 193 | 24.857 | 37.701 | -.013 | 1.00 | 16.28 | A |
| ATOM | 720 | CB | ARG | A | 193 | 23.381 | 37.591 | .372 | 1.00 | 18.72 | A |
| ATOM | 721 | CG | ARG | A | 193 | 22.590 | 36.823 | -.680 | 1.00 | 18.20 | A |
| ATOM | 722 | CD | ARG | A | 193 | 21.215 | 36.423 | -.216 | 1.00 | 21.34 | A |
| ATOM | 723 | NE | ARG | A | 193 | 20.500 | 35.721 | -1.275 | 1.00 | 20.08 | A |
| ATOM | 724 | CZ | ARG | A | 193 | 19.286 | 35.204 | -1.138 | 1.00 | 21.29 | A |
| ATOM | 725 | NH1 | ARG | A | 193 | 18.647 | 35.307 | .022 | 1.00 | 22.51 | A |
| ATOM | 726 | NH2 | ARG | A | 193 | 18.709 | 34.591 | -2.161 | 1.00 | 20.69 | A |
| ATOM | 727 | C | ARG | A | 193 | 24.997 | 38.467 | -1.314 | 1.00 | 15.74 | A |
| ATOM | 728 | O | ARG | A | 193 | 24.666 | 39.650 | -1.380 | 1.00 | 17.52 | A |
| ATOM | 729 | N | ALA | A | 194 | 25.518 | 37.798 | -2.339 | 1.00 | 13.91 | A |
| ATOM | 730 | CA | ALA | A | 194 | 25.706 | 38.422 | -3.641 | 1.00 | 15.22 | A |
| ATOM | 731 | CB | ALA | A | 194 | 26.674 | 37.593 | -4.482 | 1.00 | 13.64 | A |
| ATOM | 732 | C | ALA | A | 194 | 24.353 | 38.530 | -4.333 | 1.00 | 15.34 | A |
| ATOM | 733 | O | ALA | A | 194 | 23.612 | 37.550 | -4.424 | 1.00 | 15.21 | A |
| ATOM | 734 | N | PHE | A | 195 | 24.040 | 39.730 | -4.811 | 1.00 | 16.95 | A |
| ATOM | 735 | CA | PHE | A | 195 | 22.770 | 39.999 | -5.478 | 1.00 | 19.87 | A |
| ATOM | 736 | CB | PHE | A | 195 | 22.384 | 41.466 | -5.268 | 1.00 | 19.91 | A |
| ATOM | 737 | CG | PHE | A | 195 | 21.846 | 41.761 | -3.894 | 1.00 | 22.04 | A |
| ATOM | 738 | CD1 | PHE | A | 195 | 22.553 | 41.386 | -2.757 | 1.00 | 24.87 | A |
| ATOM | 739 | CD2 | PHE | A | 195 | 20.625 | 42.407 | -3.737 | 1.00 | 22.22 | A |
| ATOM | 740 | CE1 | PHE | A | 195 | 22.051 | 41.648 | -1.481 | 1.00 | 25.60 | A |
| ATOM | 741 | CE2 | PHE | A | 195 | 20.114 | 42.674 | -2.466 | 1.00 | 22.41 | A |
| ATOM | 742 | CZ | PHE | A | 195 | 20.829 | 42.293 | -1.337 | 1.00 | 24.45 | A |
| ATOM | 743 | C | PHE | A | 195 | 22.789 | 39.670 | -6.967 | 1.00 | 19.68 | A |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 744 | O | PHE | A | 195 | 21.758 | 39.329 | -7.550 | 1.00 | 21.50 | A |
| ATOM | 745 | N | ASN | A | 196 | 23.963 | 39.779 | -7.577 | 1.00 | 17.00 | A |
| ATOM | 746 | CA | ASN | A | 196 | 24.129 | 39.485 | -8.996 | 1.00 | 18.09 | A |
| ATOM | 747 | CB | ASN | A | 196 | 23.633 | 40.658 | -9.848 | 1.00 | 18.40 | A |
| ATOM | 748 | CG | ASN | A | 196 | 24.312 | 41.964 | -9.495 | 1.00 | 19.85 | A |
| ATOM | 749 | OD1 | ASN | A | 196 | 25.514 | 42.124 | -9.689 | 1.00 | 20.52 | A |
| ATOM | 750 | ND2 | ASN | A | 196 | 23.540 | 42.910 | -8.966 | 1.00 | 22.23 | A |
| ATOM | 751 | C | ASN | A | 196 | 25.609 | 39.218 | -9.253 | 1.00 | 16.35 | A |
| ATOM | 752 | O | ASN | A | 196 | 26.427 | 39.344 | -8.344 | 1.00 | 14.96 | A |
| ATOM | 753 | N | THR | A | 197 | 25.959 | 38.858 | -10.483 | 1.00 | 17.26 | A |
| ATOM | 754 | CA | THR | A | 197 | 27.354 | 38.557 | -10.791 | 1.00 | 16.17 | A |
| ATOM | 755 | CB | THR | A | 197 | 27.494 | 37.932 | -12.195 | 1.00 | 17.31 | A |
| ATOM | 756 | OG1 | THR | A | 197 | 26.899 | 38.793 | -13.171 | 1.00 | 20.03 | A |
| ATOM | 757 | CG2 | THR | A | 197 | 26.813 | 36.571 | -12.234 | 1.00 | 18.30 | A |
| ATOM | 758 | C | THR | A | 197 | 28.322 | 39.730 | -10.654 | 1.00 | 16.37 | A |
| ATOM | 759 | O | THR | A | 197 | 29.496 | 39.525 | -10.338 | 1.00 | 13.66 | A |
| ATOM | 760 | N | ASP | A | 198 | 27.857 | 40.956 | -10.894 | 1.00 | 16.79 | A |
| ATOM | 761 | CA | ASP | A | 198 | 28.741 | 42.107 | -10.742 | 1.00 | 18.01 | A |
| ATOM | 762 | CB | ASP | A | 198 | 28.095 | 43.394 | -11.271 | 1.00 | 22.18 | A |
| ATOM | 763 | CG | ASP | A | 198 | 28.117 | 43.486 | -12.786 | 1.00 | 26.46 | A |
| ATOM | 764 | OD1 | ASP | A | 198 | 28.972 | 42.833 | -13.420 | 1.00 | 29.30 | A |
| ATOM | 765 | OD2 | ASP | A | 198 | 27.287 | 44.235 | -13.341 | 1.00 | 31.93 | A |
| ATOM | 766 | C | ASP | A | 198 | 29.050 | 42.284 | -9.259 | 1.00 | 17.29 | A |
| ATOM | 767 | O | ASP | A | 198 | 30.197 | 42.523 | -8.874 | 1.00 | 17.00 | A |
| ATOM | 768 | N | HIS | A | 199 | 28.014 | 42.165 | -8.432 | 1.00 | 15.89 | A |
| ATOM | 769 | CA | HIS | A | 199 | 28.163 | 42.310 | -6.989 | 1.00 | 14.74 | A |
| ATOM | 770 | CB | HIS | A | 199 | 26.804 | 42.211 | -6.296 | 1.00 | 14.97 | A |
| ATOM | 771 | CG | HIS | A | 199 | 26.862 | 42.446 | -4.818 | 1.00 | 13.46 | A |
| ATOM | 772 | CD2 | HIS | A | 199 | 27.658 | 43.249 | -4.075 | 1.00 | 12.84 | A |
| ATOM | 773 | ND1 | HIS | A | 199 | 26.015 | 41.818 | -3.931 | 1.00 | 14.71 | A |
| ATOM | 774 | CE1 | HIS | A | 199 | 26.290 | 42.223 | -2.703 | 1.00 | 13.89 | A |
| ATOM | 775 | NE2 | HIS | A | 199 | 27.281 | 43.092 | -2.763 | 1.00 | 14.41 | A |
| ATOM | 776 | C | HIS | A | 199 | 29.075 | 41.211 | -6.454 | 1.00 | 13.93 | A |
| ATOM | 777 | O | HIS | A | 199 | 29.907 | 41.454 | -5.581 | 1.00 | 12.91 | A |
| ATOM | 778 | N | GLN | A | 200 | 28.902 | 40.005 | -6.985 | 1.00 | 13.22 | A |
| ATOM | 779 | CA | GLN | A | 200 | 29.702 | 38.854 | -6.573 | 1.00 | 12.96 | A |
| ATOM | 780 | CB | GLN | A | 200 | 29.331 | 37.642 | -7.421 | 1.00 | 12.31 | A |
| ATOM | 781 | CG | GLN | A | 200 | 30.026 | 36.352 | -7.013 | 1.00 | 13.47 | A |
| ATOM | 782 | CD | GLN | A | 200 | 29.566 | 35.175 | -7.848 | 1.00 | 13.16 | A |
| ATOM | 783 | OE1 | GLN | A | 200 | 28.375 | 35.028 | -8.125 | 1.00 | 15.14 | A |
| ATOM | 784 | NE2 | GLN | A | 200 | 30.504 | 34.321 | -8.245 | 1.00 | 13.84 | A |
| ATOM | 785 | C | GLN | A | 200 | 31.191 | 39.147 | -6.717 | 1.00 | 13.87 | A |
| ATOM | 786 | O | GLN | A | 200 | 31.994 | 38.816 | -5.840 | 1.00 | 12.77 | A |
| ATOM | 787 | N | THR | A | 201 | 31.556 | 39.765 | -7.834 | 1.00 | 11.64 | A |
| ATOM | 788 | CA | THR | A | 201 | 32.948 | 40.109 | -8.086 | 1.00 | 12.73 | A |
| ATOM | 789 | CB | THR | A | 201 | 33.178 | 40.403 | -9.593 | 1.00 | 11.84 | A |
| ATOM | 790 | OG1 | THR | A | 201 | 33.216 | 39.168 | -10.321 | 1.00 | 13.35 | A |
| ATOM | 791 | CG2 | THR | A | 201 | 34.479 | 41.155 | -9.803 | 1.00 | 14.26 | A |
| ATOM | 792 | C | THR | A | 201 | 33.377 | 41.313 | -7.244 | 1.00 | 11.26 | A |
| ATOM | 793 | O | THR | A | 201 | 34.495 | 41.350 | -6.727 | 1.00 | 11.94 | A |
| ATOM | 794 | N | GLN | A | 202 | 32.485 | 42.289 | -7.092 | 1.00 | 12.98 | A |
| ATOM | 795 | CA | GLN | A | 202 | 32.803 | 43.477 | -6.312 | 1.00 | 13.80 | A |
| ATOM | 796 | CB | GLN | A | 202 | 31.639 | 44.475 | -6.360 | 1.00 | 17.53 | A |
| ATOM | 797 | CG | GLN | A | 202 | 32.024 | 45.875 | -5.899 | 1.00 | 25.23 | A |
| ATOM | 798 | CD | GLN | A | 202 | 32.228 | 45.970 | -4.400 | 1.00 | 28.15 | A |
| ATOM | 799 | OE1 | GLN | A | 202 | 33.065 | 46.738 | -3.922 | 1.00 | 32.69 | A |
| ATOM | 800 | NE2 | GLN | A | 202 | 31.455 | 45.194 | -3.647 | 1.00 | 29.89 | A |
| ATOM | 801 | C | GLN | A | 202 | 33.123 | 43.115 | -4.863 | 1.00 | 12.44 | A |
| ATOM | 802 | O | GLN | A | 202 | 33.972 | 43.742 | -4.235 | 1.00 | 13.52 | A |
| ATOM | 803 | N | LEU | A | 203 | 32.449 | 42.094 | -4.342 | 1.00 | 12.46 | A |
| ATOM | 804 | CA | LEU | A | 203 | 32.672 | 41.655 | -2.968 | 1.00 | 11.73 | A |
| ATOM | 805 | CB | LEU | A | 203 | 31.704 | 40.519 | -2.608 | 1.00 | 12.52 | A |
| ATOM | 806 | CG | LEU | A | 203 | 30.257 | 40.950 | -2.332 | 1.00 | 12.51 | A |
| ATOM | 807 | CD1 | LEU | A | 203 | 29.347 | 39.739 | -2.274 | 1.00 | 14.88 | A |
| ATOM | 808 | CD2 | LEU | A | 203 | 30.204 | 41.722 | -1.023 | 1.00 | 15.21 | A |
| ATOM | 809 | C | LEU | A | 203 | 34.115 | 41.215 | -2.719 | 1.00 | 12.56 | A |
| ATOM | 810 | O | LEU | A | 203 | 34.605 | 41.288 | -1.590 | 1.00 | 11.56 | A |
| ATOM | 811 | N | LEU | A | 204 | 34.801 | 40.768 | -3.767 | 1.00 | 11.31 | A |

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| ATOM | 812 | CA | LEU | A | 204 | 36.185 | 40.339 | -3.611 | 1.00 | 11.87 | A |
| ATOM | 813 | CB | LEU | A | 204 | 36.672 | 39.614 | -4.865 | 1.00 | 11.53 | A |
| ATOM | 814 | CG | LEU | A | 204 | 35.976 | 38.285 | -5.169 | 1.00 | 12.00 | A |
| ATOM | 815 | CD1 | LEU | A | 204 | 36.753 | 37.566 | -6.269 | 1.00 | 12.14 | A |
| ATOM | 816 | CD2 | LEU | A | 204 | 35.920 | 37.417 | -3.913 | 1.00 | 12.53 | A |
| ATOM | 817 | C | LEU | A | 204 | 37.109 | 41.513 | -3.294 | 1.00 | 11.61 | A |
| ATOM | 818 | O | LEU | A | 204 | 38.158 | 41.335 | -2.679 | 1.00 | 11.18 | A |
| ATOM | 819 | N | TYR | A | 205 | 36.730 | 42.712 | -3.724 | 1.00 | 13.97 | A |
| ATOM | 820 | CA | TYR | A | 205 | 37.544 | 43.883 | -3.425 | 1.00 | 16.07 | A |
| ATOM | 821 | CB | TYR | A | 205 | 37.097 | 45.073 | -4.274 | 1.00 | 19.68 | A |
| ATOM | 822 | CG | TYR | A | 205 | 37.769 | 45.087 | -5.621 | 1.00 | 23.06 | A |
| ATOM | 823 | CD1 | TYR | A | 205 | 39.088 | 45.522 | -5.752 | 1.00 | 26.38 | A |
| ATOM | 824 | CE1 | TYR | A | 205 | 39.742 | 45.482 | -6.977 | 1.00 | 28.42 | A |
| ATOM | 825 | CD2 | TYR | A | 205 | 37.114 | 44.616 | -6.755 | 1.00 | 24.97 | A |
| ATOM | 826 | CE2 | TYR | A | 205 | 37.760 | 44.569 | -7.989 | 1.00 | 27.75 | A |
| ATOM | 827 | CZ | TYR | A | 205 | 39.073 | 45.004 | -8.091 | 1.00 | 29.20 | A |
| ATOM | 828 | OH | TYR | A | 205 | 39.722 | 44.956 | -9.304 | 1.00 | 32.07 | A |
| ATOM | 829 | C | TYR | A | 205 | 37.415 | 44.192 | -1.940 | 1.00 | 15.39 | A |
| ATOM | 830 | O | TYR | A | 205 | 38.408 | 44.484 | -1.268 | 1.00 | 14.26 | A |
| ATOM | 831 | N | GLN | A | 206 | 36.191 | 44.113 | -1.426 | 1.00 | 14.66 | A |
| ATOM | 832 | CA | GLN | A | 206 | 35.957 | 44.355 | -.007 | 1.00 | 14.18 | A |
| ATOM | 833 | CB | GLN | A | 206 | 34.459 | 44.298 | .310 | 1.00 | 16.50 | A |
| ATOM | 834 | CG | GLN | A | 206 | 33.621 | 45.297 | -.469 | 1.00 | 21.42 | A |
| ATOM | 835 | CD | GLN | A | 206 | 32.151 | 45.230 | -.103 | 1.00 | 24.13 | A |
| ATOM | 836 | OE1 | GLN | A | 206 | 31.282 | 45.253 | -.975 | 1.00 | 26.96 | A |
| ATOM | 837 | NE2 | GLN | A | 206 | 31.863 | 45.156 | 1.193 | 1.00 | 26.12 | A |
| ATOM | 838 | C | GLN | A | 206 | 36.682 | 43.262 | .768 | 1.00 | 11.99 | A |
| ATOM | 839 | O | GLN | A | 206 | 37.325 | 43.520 | 1.784 | 1.00 | 13.05 | A |
| ATOM | 840 | N | ALA | A | 207 | 36.577 | 42.033 | .276 | 1.00 | 11.37 | A |
| ATOM | 841 | CA | ALA | A | 207 | 37.224 | 40.901 | .924 | 1.00 | 9.55 | A |
| ATOM | 842 | CB | ALA | A | 207 | 36.981 | 39.630 | .112 | 1.00 | 11.15 | A |
| ATOM | 843 | C | ALA | A | 207 | 38.726 | 41.137 | 1.086 | 1.00 | 9.68 | A |
| ATOM | 844 | O | ALA | A | 207 | 39.286 | 40.901 | 2.154 | 1.00 | 10.32 | A |
| ATOM | 845 | N | SER | | 208 | 39.370 | 41.607 | .021 | .50 | 8.91 | AC1 |
| ATOM | 846 | CA | SER | | 208 | 40.809 | 41.855 | .055 | .50 | 8.84 | AC1 |
| ATOM | 847 | CB | SER | | 208 | 41.319 | 42.271 | -1.332 | .50 | 8.15 | AC1 |
| ATOM | 848 | OG | SER | | 208 | 40.748 | 43.489 | -1.778 | .50 | 5.66 | AC1 |
| ATOM | 849 | C | SER | | 208 | 41.180 | 42.910 | 1.091 | .50 | 8.91 | AC1 |
| ATOM | 850 | O | SER | | 208 | 42.186 | 42.773 | 1.787 | .50 | 9.06 | AC1 |
| ATOM | 851 | N | ALA | A | 209 | 40.364 | 43.955 | 1.198 | 1.00 | 9.46 | A |
| ATOM | 852 | CA | ALA | A | 209 | 40.613 | 45.020 | 2.163 | 1.00 | 10.03 | A |
| ATOM | 853 | CB | ALA | A | 209 | 39.631 | 46.163 | 1.940 | 1.00 | 11.01 | A |
| ATOM | 854 | C | ALA | A | 209 | 40.474 | 44.466 | 3.581 | 1.00 | 12.23 | A |
| ATOM | 855 | O | ALA | A | 209 | 41.252 | 44.796 | 4.474 | 1.00 | 13.45 | A |
| ATOM | 856 | N | MSE | A | 210 | 39.483 | 43.608 | 3.782 | 1.00 | 11.13 | A |
| ATOM | 857 | CA | MSE | A | 210 | 39.263 | 43.015 | 5.093 | 1.00 | 11.31 | A |
| ATOM | 858 | CB | MSE | A | 210 | 37.939 | 42.245 | 5.087 | 1.00 | 11.10 | A |
| ATOM | 859 | CG | MSE | A | 210 | 36.738 | 43.163 | 4.929 | 1.00 | 12.90 | A |
| ATOM | 860 | SE | MSE | A | 210 | 35.166 | 42.285 | 4.275 | 1.00 | 19.56 | A |
| ATOM | 861 | CE | MSE | A | 210 | 34.748 | 41.258 | 5.846 | 1.00 | 18.08 | A |
| ATOM | 862 | C | MSE | A | 210 | 40.416 | 42.100 | 5.502 | 1.00 | 10.40 | A |
| ATOM | 863 | O | MSE | A | 210 | 40.816 | 42.075 | 6.667 | 1.00 | 11.49 | A |
| ATOM | 864 | N | MSE | A | 211 | 40.959 | 41.361 | 4.538 | 1.00 | 9.79 | A |
| ATOM | 865 | CA | MSE | A | 211 | 42.054 | 40.442 | 4.809 | 1.00 | 9.90 | A |
| ATOM | 866 | CB | MSE | A | 211 | 42.246 | 39.502 | 3.622 | 1.00 | 11.35 | A |
| ATOM | 867 | CG | MSE | A | 211 | 41.034 | 38.605 | 3.419 | 1.00 | 13.28 | A |
| ATOM | 868 | SE | MSE | A | 211 | 41.249 | 37.350 | 1.970 | 1.00 | 19.97 | A |
| ATOM | 869 | CE | MSE | A | 211 | 39.669 | 36.267 | 2.266 | 1.00 | 17.37 | A |
| ATOM | 870 | C | MSE | A | 211 | 43.354 | 41.161 | 5.150 | 1.00 | 12.40 | A |
| ATOM | 871 | O | MSE | A | 211 | 44.254 | 40.576 | 5.751 | 1.00 | 12.31 | A |
| ATOM | 872 | N | VAL | A | 212 | 43.448 | 42.429 | 4.771 | 1.00 | 13.63 | A |
| ATOM | 873 | CA | VAL | A | 212 | 44.633 | 43.219 | 5.092 | 1.00 | 16.42 | A |
| ATOM | 874 | CB | VAL | A | 212 | 44.710 | 44.499 | 4.215 | 1.00 | 16.91 | A |
| ATOM | 875 | CG1 | VAL | A | 212 | 45.666 | 45.507 | 4.837 | 1.00 | 20.67 | A |
| ATOM | 876 | CG2 | VAL | A | 212 | 45.179 | 44.141 | 2.815 | 1.00 | 16.11 | A |
| ATOM | 877 | C | VAL | A | 212 | 44.566 | 43.633 | 6.565 | 1.00 | 18.07 | A |
| ATOM | 878 | O | VAL | A | 212 | 45.587 | 43.696 | 7.256 | 1.00 | 20.15 | A |
| ATOM | 879 | N | GLU | A | 213 | 43.351 | 43.890 | 7.039 | 1.00 | 17.71 | A |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 880 | CA | GLU | A | 213 | 43.111 | 44.333 | 8.412 | 1.00 | 19.16 | A |
| ATOM | 881 | CB | GLU | A | 213 | 41.801 | 45.127 | 8.470 | 1.00 | 21.15 | A |
| ATOM | 882 | CG | GLU | A | 213 | 41.862 | 46.502 | 7.823 | 1.00 | 24.58 | A |
| ATOM | 883 | CD | GLU | A | 213 | 40.552 | 47.263 | 7.955 | 1.00 | 28.91 | A |
| ATOM | 884 | OE1 | GLU | A | 213 | 39.820 | 47.024 | 8.940 | 1.00 | 29.96 | A |
| ATOM | 885 | OE2 | GLU | A | 213 | 40.257 | 48.111 | 7.085 | 1.00 | 30.33 | A |
| ATOM | 886 | C | GLU | A | 213 | 43.076 | 43.256 | 9.498 | 1.00 | 19.63 | A |
| ATOM | 887 | O | GLU | A | 213 | 43.546 | 43.486 | 10.614 | 1.00 | 18.83 | A |
| ATOM | 888 | N | SER | A | 214 | 42.509 | 42.093 | 9.184 | 1.00 | 18.76 | A |
| ATOM | 889 | CA | SER | A | 214 | 42.399 | 41.004 | 10.159 | 1.00 | 18.30 | A |
| ATOM | 890 | CB | SER | A | 214 | 40.945 | 40.857 | 10.626 | 1.00 | 20.42 | A |
| ATOM | 891 | OG | SER | A | 214 | 40.397 | 42.099 | 11.016 | 1.00 | 25.34 | A |
| ATOM | 892 | C | SER | A | 214 | 42.839 | 39.686 | 9.546 | 1.00 | 17.21 | A |
| ATOM | 893 | O | SER | A | 214 | 42.840 | 39.540 | 8.324 | 1.00 | 15.90 | A |
| ATOM | 894 | N | ARG | A | 215 | 43.190 | 38.719 | 10.391 | 1.00 | 16.03 | A |
| ATOM | 895 | CA | ARG | A | 215 | 43.612 | 37.419 | 9.891 | 1.00 | 14.50 | A |
| ATOM | 896 | CB | ARG | A | 215 | 44.521 | 36.686 | 10.885 | 1.00 | 17.55 | A |
| ATOM | 897 | CG | ARG | A | 215 | 44.837 | 35.257 | 10.414 | 1.00 | 20.04 | A |
| ATOM | 898 | CD | ARG | A | 215 | 45.692 | 34.456 | 11.384 | 1.00 | 25.67 | A |
| ATOM | 899 | NE | ARG | A | 215 | 45.705 | 33.035 | 11.032 | 1.00 | 28.44 | A |
| ATOM | 900 | CZ | ARG | A | 215 | 46.186 | 32.539 | 9.894 | 1.00 | 32.44 | A |
| ATOM | 901 | NH1 | ARG | A | 215 | 46.710 | 33.342 | 8.977 | 1.00 | 33.60 | A |
| ATOM | 902 | NH2 | ARG | A | 215 | 46.132 | 31.232 | 9.664 | 1.00 | 33.47 | A |
| ATOM | 903 | C | ARG | A | 215 | 42.444 | 36.502 | 9.568 | 1.00 | 13.33 | A |
| ATOM | 904 | O | ARG | A | 215 | 41.666 | 36.124 | 10.448 | 1.00 | 14.15 | A |
| ATOM | 905 | N | TYR | A | 216 | 42.337 | 36.148 | 8.294 | 1.00 | 12.11 | A |
| ATOM | 906 | CA | TYR | A | 216 | 41.309 | 35.235 | 7.826 | 1.00 | 10.66 | A |
| ATOM | 907 | CB | TYR | A | 216 | 40.597 | 35.796 | 6.600 | 1.00 | 11.82 | A |
| ATOM | 908 | CG | TYR | A | 216 | 39.502 | 36.761 | 6.941 | 1.00 | 11.74 | A |
| ATOM | 909 | CD1 | TYR | A | 216 | 39.789 | 38.074 | 7.311 | 1.00 | 13.91 | A |
| ATOM | 910 | CE1 | TYR | A | 216 | 38.773 | 38.950 | 7.670 | 1.00 | 14.14 | A |
| ATOM | 911 | CD2 | TYR | A | 216 | 38.172 | 36.348 | 6.939 | 1.00 | 13.07 | A |
| ATOM | 912 | CE2 | TYR | A | 216 | 37.157 | 37.209 | 7.296 | 1.00 | 13.62 | A |
| ATOM | 913 | CZ | TYR | A | 216 | 37.459 | 38.506 | 7.661 | 1.00 | 15.01 | A |
| ATOM | 914 | OH | TYR | A | 216 | 36.434 | 39.349 | 8.016 | 1.00 | 17.98 | A |
| ATOM | 915 | C | TYR | A | 216 | 41.996 | 33.942 | 7.435 | 1.00 | 10.55 | A |
| ATOM | 916 | O | TYR | A | 216 | 43.151 | 33.952 | 7.012 | 1.00 | 11.94 | A |
| ATOM | 917 | N | ALA | A | 217 | 41.288 | 32.829 | 7.572 | 1.00 | 8.82 | A |
| ATOM | 918 | CA | ALA | A | 217 | 41.849 | 31.538 | 7.200 | 1.00 | 8.08 | A |
| ATOM | 919 | CB | ALA | A | 217 | 41.849 | 30.599 | 8.403 | 1.00 | 10.40 | A |
| ATOM | 920 | C | ALA | A | 217 | 41.023 | 30.927 | 6.082 | 1.00 | 8.74 | A |
| ATOM | 921 | O | ALA | A | 217 | 41.492 | 30.030 | 5.380 | 1.00 | 9.17 | A |
| ATOM | 922 | N | LEU | A | 218 | 39.811 | 31.440 | 5.889 | 1.00 | 8.26 | A |
| ATOM | 923 | CA | LEU | A | 218 | 38.913 | 30.856 | 4.897 | 1.00 | 9.02 | A |
| ATOM | 924 | CB | LEU | A | 218 | 38.089 | 29.765 | 5.593 | 1.00 | 9.51 | A |
| ATOM | 925 | CG | LEU | A | 218 | 36.917 | 29.094 | 4.872 | 1.00 | 10.64 | A |
| ATOM | 926 | CD1 | LEU | A | 218 | 37.450 | 28.079 | 3.870 | 1.00 | 11.06 | A |
| ATOM | 927 | CD2 | LEU | A | 218 | 36.024 | 28.398 | 5.892 | 1.00 | 13.12 | A |
| ATOM | 928 | C | LEU | A | 218 | 37.946 | 31.799 | 4.184 | 1.00 | 7.66 | A |
| ATOM | 929 | O | LEU | A | 218 | 37.368 | 32.697 | 4.794 | 1.00 | 8.43 | A |
| ATOM | 930 | N | LEU | A | 219 | 37.778 | 31.571 | 2.885 | 1.00 | 8.37 | A |
| ATOM | 931 | CA | LEU | A | 219 | 36.821 | 32.322 | 2.078 | 1.00 | 7.10 | A |
| ATOM | 932 | CB | LEU | A | 219 | 37.507 | 33.171 | 1.000 | 1.00 | 9.27 | A |
| ATOM | 933 | CG | LEU | A | 219 | 36.542 | 33.707 | -.075 | 1.00 | 10.99 | A |
| ATOM | 934 | CD1 | LEU | A | 219 | 35.445 | 34.564 | .560 | 1.00 | 13.35 | A |
| ATOM | 935 | CD2 | LEU | A | 219 | 37.322 | 34.518 | -1.101 | 1.00 | 12.85 | A |
| ATOM | 936 | C | LEU | A | 219 | 35.929 | 31.294 | 1.395 | 1.00 | 7.22 | A |
| ATOM | 937 | O | LEU | A | 219 | 36.412 | 30.419 | .668 | 1.00 | 7.85 | A |
| ATOM | 938 | N | ILE | | 220 | 34.627 | 31.412 | 1.626 | .50 | 6.12 | AC1 |
| ATOM | 939 | CA | ILE | | 220 | 33.644 | 30.508 | 1.045 | .50 | 5.48 | AC1 |
| ATOM | 940 | CB | ILE | | 220 | 32.706 | 29.953 | 2.131 | .50 | 5.16 | AC1 |
| ATOM | 941 | CG2 | ILE | | 220 | 31.606 | 29.110 | 1.492 | .50 | 5.91 | AC1 |
| ATOM | 942 | CG1 | ILE | | 220 | 33.509 | 29.143 | 3.150 | .50 | 4.87 | AC1 |
| ATOM | 943 | CD1 | ILE | | 220 | 32.776 | 28.924 | 4.455 | .50 | 2.48 | AC1 |
| ATOM | 944 | C | ILE | | 220 | 32.785 | 31.247 | .029 | .50 | 5.49 | AC1 |
| ATOM | 945 | O | ILE | | 220 | 32.343 | 32.369 | .281 | .50 | 5.14 | AC1 |
| ATOM | 946 | N | VAL | A | 221 | 32.555 | 30.616 | -1.118 | 1.00 | 6.21 | A |
| ATOM | 947 | CA | VAL | A | 221 | 31.713 | 31.202 | -2.158 | 1.00 | 6.05 | A |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 948 | CB | VAL | A | 221 | 32.479 | 31.630 | -3.418 | 1.00 | 8.43 | A |
| ATOM | 949 | CG1 | VAL | A | 221 | 31.489 | 32.232 | -4.424 | 1.00 | 11.56 | A |
| ATOM | 950 | CG2 | VAL | A | 221 | 33.545 | 32.652 | -3.065 | 1.00 | 9.56 | A |
| ATOM | 951 | C | VAL | A | 221 | 30.747 | 30.083 | -2.525 | 1.00 | 9.19 | A |
| ATOM | 952 | O | VAL | A | 221 | 31.097 | 29.156 | -3.257 | 1.00 | 9.66 | A |
| ATOM | 953 | N | ASP | A | 222 | 29.530 | 30.182 | -2.001 | 1.00 | 8.99 | A |
| ATOM | 954 | CA | ASP | A | 222 | 28.488 | 29.178 | -2.208 | 1.00 | 10.19 | A |
| ATOM | 955 | CB | ASP | A | 222 | 28.237 | 28.482 | -.859 | 1.00 | 12.30 | A |
| ATOM | 956 | CG | ASP | A | 222 | 27.093 | 27.492 | -.899 | 1.00 | 13.65 | A |
| ATOM | 957 | OD1 | ASP | A | 222 | 26.893 | 26.851 | -1.945 | 1.00 | 14.21 | A |
| ATOM | 958 | OD2 | ASP | A | 222 | 26.407 | 27.343 | .138 | 1.00 | 17.00 | A |
| ATOM | 959 | C | ASP | A | 222 | 27.218 | 29.870 | -2.712 | 1.00 | 10.73 | A |
| ATOM | 960 | O | ASP | A | 222 | 26.485 | 30.447 | -1.914 | 1.00 | 11.04 | A |
| ATOM | 961 | N | SER | A | 223 | 26.926 | 29.815 | -4.014 | 1.00 | 11.76 | A |
| ATOM | 962 | CA | SER | A | 223 | 27.693 | 29.127 | -5.053 | 1.00 | 11.53 | A |
| ATOM | 963 | CB | SER | A | 223 | 26.717 | 28.320 | -5.922 | 1.00 | 13.99 | A |
| ATOM | 964 | OG | SER | A | 223 | 27.250 | 28.040 | -7.204 | 1.00 | 15.91 | A |
| ATOM | 965 | C | SER | A | 223 | 28.470 | 30.107 | -5.937 | 1.00 | 12.18 | A |
| ATOM | 966 | O | SER | A | 223 | 28.063 | 31.256 | -6.113 | 1.00 | 12.29 | A |
| ATOM | 967 | N | ALA | A | 224 | 29.578 | 29.649 | -6.509 | 1.00 | 11.55 | A |
| ATOM | 968 | CA | ALA | A | 224 | 30.389 | 30.505 | -7.365 | 1.00 | 12.08 | A |
| ATOM | 969 | CB | ALA | A | 224 | 31.815 | 29.960 | -7.447 | 1.00 | 12.08 | A |
| ATOM | 970 | C | ALA | A | 224 | 29.812 | 30.646 | -8.771 | 1.00 | 12.99 | A |
| ATOM | 971 | O | ALA | A | 224 | 30.159 | 31.578 | -9.495 | 1.00 | 13.90 | A |
| ATOM | 972 | N | THR | A | 225 | 28.916 | 29.741 | -9.150 | 1.00 | 14.01 | A |
| ATOM | 973 | CA | THR | A | 225 | 28.355 | 29.777 | -10.497 | 1.00 | 15.06 | A |
| ATOM | 974 | CB | THR | A | 225 | 28.715 | 28.492 | -11.251 | 1.00 | 15.67 | A |
| ATOM | 975 | OG1 | THR | A | 225 | 28.169 | 27.367 | -10.550 | 1.00 | 18.32 | A |
| ATOM | 976 | CG2 | THR | A | 225 | 30.227 | 28.341 | -11.350 | 1.00 | 17.70 | A |
| ATOM | 977 | C | THR | A | 225 | 26.844 | 29.966 | -10.621 | 1.00 | 16.24 | A |
| ATOM | 978 | O | THR | A | 225 | 26.353 | 30.310 | -11.696 | 1.00 | 16.22 | A |
| ATOM | 979 | N | ALA | A | 226 | 26.111 | 29.742 | -9.536 | 1.00 | 15.40 | A |
| ATOM | 980 | CA | ALA | A | 226 | 24.655 | 29.863 | -9.569 | 1.00 | 17.16 | A |
| ATOM | 981 | CB | ALA | A | 226 | 24.087 | 29.724 | -8.157 | 1.00 | 17.20 | A |
| ATOM | 982 | C | ALA | A | 226 | 24.121 | 31.139 | -10.218 | 1.00 | 18.11 | A |
| ATOM | 983 | O | ALA | A | 226 | 23.215 | 31.080 | -11.050 | 1.00 | 19.76 | A |
| ATOM | 984 | N | LEU | A | 227 | 24.677 | 32.289 | -9.849 | 1.00 | 17.52 | A |
| ATOM | 985 | CA | LEU | A | 227 | 24.207 | 33.558 | -10.396 | 1.00 | 17.98 | A |
| ATOM | 986 | CB | LEU | A | 227 | 24.802 | 34.726 | -9.603 | 1.00 | 18.01 | A |
| ATOM | 987 | CG | LEU | A | 227 | 24.397 | 34.787 | -8.123 | 1.00 | 18.20 | A |
| ATOM | 988 | CD1 | LEU | A | 227 | 24.978 | 36.043 | -7.489 | 1.00 | 19.48 | A |
| ATOM | 989 | CD2 | LEU | A | 227 | 22.876 | 34.783 | -7.992 | 1.00 | 21.19 | A |
| ATOM | 990 | C | LEU | A | 227 | 24.481 | 33.740 | -11.890 | 1.00 | 18.80 | A |
| ATOM | 991 | O | LEU | A | 227 | 23.895 | 34.616 | -12.530 | 1.00 | 18.94 | A |
| ATOM | 992 | N | TYR | A | 228 | 25.360 | 32.911 | -12.443 | 1.00 | 18.50 | A |
| ATOM | 993 | CA | TYR | A | 228 | 25.693 | 32.986 | -13.863 | 1.00 | 21.58 | A |
| ATOM | 994 | CB | TYR | A | 228 | 27.107 | 32.450 | -14.099 | 1.00 | 17.41 | A |
| ATOM | 995 | CG | TYR | A | 228 | 28.196 | 33.411 | -13.689 | 1.00 | 14.92 | A |
| ATOM | 996 | CD1 | TYR | A | 228 | 28.626 | 34.417 | -14.554 | 1.00 | 12.76 | A |
| ATOM | 997 | CE1 | TYR | A | 228 | 29.620 | 35.314 | -14.179 | 1.00 | 13.80 | A |
| ATOM | 998 | CD2 | TYR | A | 228 | 28.789 | 33.328 | -12.430 | 1.00 | 13.04 | A |
| ATOM | 999 | CE2 | TYR | A | 228 | 29.785 | 34.224 | -12.044 | 1.00 | 12.87 | A |
| ATOM | 1000 | CZ | TYR | A | 228 | 30.196 | 35.211 | -12.920 | 1.00 | 12.36 | A |
| ATOM | 1001 | OH | TYR | A | 228 | 31.182 | 36.091 | -12.551 | 1.00 | 14.32 | A |
| ATOM | 1002 | C | TYR | A | 228 | 24.699 | 32.205 | -14.717 | 1.00 | 25.16 | A |
| ATOM | 1003 | O | TYR | A | 228 | 24.694 | 32.327 | -15.942 | 1.00 | 27.01 | A |
| ATOM | 1004 | N | ARG | A | 229 | 23.857 | 31.409 | -14.066 | 1.00 | 28.73 | A |
| ATOM | 1005 | CA | ARG | A | 229 | 22.861 | 30.608 | -14.770 | 1.00 | 34.06 | A |
| ATOM | 1006 | CB | ARG | A | 229 | 22.862 | 29.173 | -14.233 | 1.00 | 37.97 | A |
| ATOM | 1007 | CG | ARG | A | 229 | 21.948 | 28.221 | -14.994 | 1.00 | 45.76 | A |
| ATOM | 1008 | CD | ARG | A | 229 | 22.082 | 26.795 | -14.476 | 1.00 | 50.57 | A |
| ATOM | 1009 | NE | ARG | A | 229 | 21.591 | 26.658 | -13.107 | 1.00 | 56.15 | A |
| ATOM | 1010 | CZ | ARG | A | 229 | 20.304 | 26.628 | -12.771 | 1.00 | 58.13 | A |
| ATOM | 1011 | NH1 | ARG | A | 229 | 19.366 | 26.723 | -13.705 | 1.00 | 59.34 | A |
| ATOM | 1012 | NH2 | ARG | A | 229 | 19.955 | 26.504 | -11.498 | 1.00 | 59.67 | A |
| ATOM | 1013 | C | ARG | A | 229 | 21.469 | 31.210 | -14.619 | 1.00 | 35.05 | A |
| ATOM | 1014 | O | ARG | A | 229 | 21.162 | 32.242 | -15.216 | 1.00 | 37.10 | A |
| ATOM | 1015 | N | GLU | A | 237 | 26.455 | 36.730 | -25.203 | 1.00 | 45.75 | A |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1016 | CA | GLU | A | 237 | 25.871 | 36.676 | -23.870 | 1.00 | 45.26 | A |
| ATOM | 1017 | CB | GLU | A | 237 | 24.361 | 36.455 | -23.965 | 1.00 | 47.65 | A |
| ATOM | 1018 | CG | GLU | A | 237 | 23.661 | 36.374 | -22.618 | 1.00 | 51.11 | A |
| ATOM | 1019 | CD | GLU | A | 237 | 24.004 | 37.545 | -21.718 | 1.00 | 52.82 | A |
| ATOM | 1020 | OE1 | GLU | A | 237 | 23.878 | 38.701 | -22.172 | 1.00 | 54.95 | A |
| ATOM | 1021 | OE2 | GLU | A | 237 | 24.397 | 37.309 | -20.555 | 1.00 | 53.95 | A |
| ATOM | 1022 | C | GLU | A | 237 | 26.505 | 35.558 | -23.052 | 1.00 | 43.96 | A |
| ATOM | 1023 | O | GLU | A | 237 | 27.098 | 35.803 | -22.001 | 1.00 | 43.47 | A |
| ATOM | 1024 | N | LEU | A | 238 | 26.371 | 34.329 | -23.541 | 1.00 | 41.51 | A |
| ATOM | 1025 | CA | LEU | A | 238 | 26.937 | 33.170 | -22.866 | 1.00 | 39.97 | A |
| ATOM | 1026 | CB | LEU | A | 238 | 26.619 | 31.896 | -23.650 | 1.00 | 41.06 | A |
| ATOM | 1027 | CG | LEU | A | 238 | 27.342 | 30.621 | -23.203 | 1.00 | 42.05 | A |
| ATOM | 1028 | CD1 | LEU | A | 238 | 27.008 | 30.309 | -21.751 | 1.00 | 42.90 | A |
| ATOM | 1029 | CD2 | LEU | A | 238 | 26.935 | 29.469 | -24.107 | 1.00 | 43.61 | A |
| ATOM | 1030 | C | LEU | A | 238 | 28.447 | 33.318 | -22.725 | 1.00 | 38.07 | A |
| ATOM | 1031 | O | LEU | A | 238 | 29.005 | 33.095 | -21.651 | 1.00 | 36.76 | A |
| ATOM | 1032 | N | SER | A | 239 | 29.105 | 33.693 | -23.818 | 1.00 | 35.69 | A |
| ATOM | 1033 | CA | SER | A | 239 | 30.552 | 33.870 | -23.813 | 1.00 | 33.46 | A |
| ATOM | 1034 | CB | SER | A | 239 | 31.055 | 34.167 | -25.227 | 1.00 | 34.80 | A |
| ATOM | 1035 | OG | SER | A | 239 | 30.508 | 35.377 | -25.721 | 1.00 | 37.47 | A |
| ATOM | 1036 | C | SER | A | 239 | 30.947 | 35.005 | -22.875 | 1.00 | 31.86 | A |
| ATOM | 1037 | O | SER | A | 239 | 32.013 | 34.973 | -22.260 | 1.00 | 30.28 | A |
| ATOM | 1038 | N | ALA | A | 240 | 30.082 | 36.008 | -22.769 | 1.00 | 29.26 | A |
| ATOM | 1039 | CA | ALA | A | 240 | 30.344 | 37.146 | -21.897 | 1.00 | 27.57 | A |
| ATOM | 1040 | CB | ALA | A | 240 | 29.276 | 38.212 | -22.091 | 1.00 | 28.86 | A |
| ATOM | 1041 | C | ALA | A | 240 | 30.359 | 36.676 | -20.446 | 1.00 | 26.33 | A |
| ATOM | 1042 | O | ALA | A | 240 | 31.229 | 37.065 | -19.665 | 1.00 | 24.83 | A |
| ATOM | 1043 | N | ARG | A | 241 | 29.391 | 35.837 | -20.095 | 1.00 | 24.47 | A |
| ATOM | 1044 | CA | ARG | A | 241 | 29.298 | 35.308 | -18.741 | 1.00 | 24.64 | A |
| ATOM | 1045 | CB | ARG | A | 241 | 27.986 | 34.545 | -18.545 | 1.00 | 26.26 | A |
| ATOM | 1046 | CG | ARG | A | 241 | 26.748 | 35.415 | -18.618 | 1.00 | 30.40 | A |
| ATOM | 1047 | CD | ARG | A | 241 | 25.509 | 34.636 | -18.222 | 1.00 | 32.71 | A |
| ATOM | 1048 | NE | ARG | A | 241 | 24.309 | 35.459 | -18.327 | 1.00 | 37.68 | A |
| ATOM | 1049 | CZ | ARG | A | 241 | 23.094 | 35.063 | -17.964 | 1.00 | 40.61 | A |
| ATOM | 1050 | NH1 | ARG | A | 241 | 22.910 | 33.848 | -17.465 | 1.00 | 42.19 | A |
| ATOM | 1051 | NH2 | ARG | A | 241 | 22.061 | 35.883 | -18.104 | 1.00 | 41.34 | A |
| ATOM | 1052 | C | ARG | A | 241 | 30.467 | 34.381 | -18.436 | 1.00 | 23.05 | A |
| ATOM | 1053 | O | ARG | A | 241 | 30.986 | 34.376 | -17.321 | 1.00 | 21.52 | A |
| ATOM | 1054 | N | GLN | A | 242 | 30.882 | 33.597 | -19.427 | 1.00 | 21.32 | A |
| ATOM | 1055 | CA | GLN | A | 242 | 31.991 | 32.675 | -19.227 | 1.00 | 22.07 | A |
| ATOM | 1056 | CB | GLN | A | 242 | 32.152 | 31.754 | -20.442 | 1.00 | 26.14 | A |
| ATOM | 1057 | CG | GLN | A | 242 | 31.006 | 30.759 | -20.591 | 1.00 | 32.63 | A |
| ATOM | 1058 | CD | GLN | A | 242 | 31.207 | 29.788 | -21.737 | 1.00 | 37.09 | A |
| ATOM | 1059 | OE1 | GLN | A | 242 | 31.310 | 30.188 | -22.897 | 1.00 | 39.23 | A |
| ATOM | 1060 | NE2 | GLN | A | 242 | 31.259 | 28.499 | -21.415 | 1.00 | 39.89 | A |
| ATOM | 1061 | C | GLN | A | 242 | 33.291 | 33.417 | -18.946 | 1.00 | 19.58 | A |
| ATOM | 1062 | O | GLN | A | 242 | 34.074 | 32.992 | -18.098 | 1.00 | 17.88 | A |
| ATOM | 1063 | N | MSE | A | 243 | 33.519 | 34.521 | -19.652 | 1.00 | 18.13 | A |
| ATOM | 1064 | CA | MSE | A | 243 | 34.729 | 35.313 | -19.444 | 1.00 | 18.31 | A |
| ATOM | 1065 | CB | MSE | A | 243 | 34.868 | 36.397 | -20.519 | 1.00 | 20.88 | A |
| ATOM | 1066 | CG | MSE | A | 243 | 35.243 | 35.872 | -21.895 | 1.00 | 24.97 | A |
| ATOM | 1067 | SE | MSE | A | 243 | 35.643 | 37.308 | -23.133 | 1.00 | 31.39 | A |
| ATOM | 1068 | CE | MSE | A | 243 | 33.856 | 37.603 | -23.805 | 1.00 | 31.87 | A |
| ATOM | 1069 | C | MSE | A | 243 | 34.701 | 35.976 | -18.073 | 1.00 | 17.43 | A |
| ATOM | 1070 | O | MSE | A | 243 | 35.715 | 36.041 | -17.384 | 1.00 | 15.93 | A |
| ATOM | 1071 | N | HIS | A | 244 | 33.532 | 36.473 | -17.684 | 1.00 | 15.35 | A |
| ATOM | 1072 | CA | HIS | A | 244 | 33.382 | 37.135 | -16.396 | 1.00 | 14.53 | A |
| ATOM | 1073 | CB | HIS | A | 244 | 31.975 | 37.732 | -16.286 | 1.00 | 16.88 | A |
| ATOM | 1074 | CG | HIS | A | 244 | 31.813 | 38.698 | -15.155 | 1.00 | 18.28 | A |
| ATOM | 1075 | CD2 | HIS | A | 244 | 31.863 | 40.050 | -15.125 | 1.00 | 17.28 | A |
| ATOM | 1076 | ND1 | HIS | A | 244 | 31.585 | 38.294 | -13.857 | 1.00 | 17.51 | A |
| ATOM | 1077 | CE1 | HIS | A | 244 | 31.502 | 39.355 | -13.076 | 1.00 | 17.03 | A |
| ATOM | 1078 | NE2 | HIS | A | 244 | 31.667 | 40.435 | -13.820 | 1.00 | 18.85 | A |
| ATOM | 1079 | C | HIS | A | 244 | 33.645 | 36.141 | -15.264 | 1.00 | 13.42 | A |
| ATOM | 1080 | O | HIS | A | 244 | 34.323 | 36.466 | -14.290 | 1.00 | 11.85 | A |
| ATOM | 1081 | N | LEU | A | 245 | 33.111 | 34.931 | -15.400 | 1.00 | 12.32 | A |
| ATOM | 1082 | CA | LEU | A | 245 | 33.313 | 33.894 | -14.393 | 1.00 | 11.41 | A |
| ATOM | 1083 | CB | LEU | A | 245 | 32.459 | 32.664 | -14.716 | 1.00 | 11.93 | A |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1084 | CG | LEU | A | 245 | 32.704 | 31.410 | -13.869 | 1.00 | 12.45 | A |
| ATOM | 1085 | CD1 | LEU | A | 245 | 32.472 | 31.715 | -12.389 | 1.00 | 12.44 | A |
| ATOM | 1086 | CD2 | LEU | A | 245 | 31.778 | 30.300 | -14.339 | 1.00 | 13.60 | A |
| ATOM | 1087 | C | LEU | A | 245 | 34.790 | 33.504 | -14.341 | 1.00 | 11.45 | A |
| ATOM | 1088 | O | LEU | A | 245 | 35.363 | 33.358 | -13.263 | 1.00 | 11.37 | A |
| ATOM | 1089 | N | ALA | A | 246 | 35.411 | 33.344 | -15.506 | 1.00 | 11.75 | A |
| ATOM | 1090 | CA | ALA | A | 246 | 36.822 | 32.976 | -15.558 | 1.00 | 11.29 | A |
| ATOM | 1091 | CB | ALA | A | 246 | 37.298 | 32.895 | -17.007 | 1.00 | 11.67 | A |
| ATOM | 1092 | C | ALA | A | 246 | 37.655 | 33.998 | -14.791 | 1.00 | 11.07 | A |
| ATOM | 1093 | O | ALA | A | 246 | 38.552 | 33.638 | -14.032 | 1.00 | 10.62 | A |
| ATOM | 1094 | N | ARG | A | 247 | 37.344 | 35.274 | -14.985 | 1.00 | 11.10 | A |
| ATOM | 1095 | CA | ARG | A | 247 | 38.064 | 36.337 | -14.300 | 1.00 | 12.88 | A |
| ATOM | 1096 | CB | ARG | A | 247 | 37.572 | 37.702 | -14.774 | 1.00 | 17.27 | A |
| ATOM | 1097 | CG | ARG | A | 247 | 38.347 | 38.868 | -14.189 | 1.00 | 25.65 | A |
| ATOM | 1098 | CD | ARG | A | 247 | 39.732 | 38.971 | -14.804 | 1.00 | 32.96 | A |
| ATOM | 1099 | NE | ARG | A | 247 | 40.475 | 40.118 | -14.287 | 1.00 | 39.20 | A |
| ATOM | 1100 | CZ | ARG | A | 247 | 41.244 | 40.089 | -13.204 | 1.00 | 41.96 | A |
| ATOM | 1101 | NH1 | ARG | A | 247 | 41.387 | 38.965 | -12.512 | 1.00 | 42.95 | A |
| ATOM | 1102 | NH2 | ARG | A | 247 | 41.862 | 41.192 | -12.807 | 1.00 | 43.69 | A |
| ATOM | 1103 | C | ARG | A | 247 | 37.841 | 36.204 | -12.795 | 1.00 | 11.48 | A |
| ATOM | 1104 | O | ARG | A | 247 | 38.779 | 36.316 | -12.005 | 1.00 | 11.35 | A |
| ATOM | 1105 | N | PHE | A | 248 | 36.591 | 35.971 | -12.406 | 1.00 | 9.96 | A |
| ATOM | 1106 | CA | PHE | A | 248 | 36.257 | 35.809 | -10.993 | 1.00 | 8.76 | A |
| ATOM | 1107 | CB | PHE | A | 248 | 34.775 | 35.465 | -10.831 | 1.00 | 8.82 | A |
| ATOM | 1108 | CG | PHE | A | 248 | 34.360 | 35.228 | -9.402 | 1.00 | 8.05 | A |
| ATOM | 1109 | CD1 | PHE | A | 248 | 34.228 | 36.293 | -8.515 | 1.00 | 9.83 | A |
| ATOM | 1110 | CD2 | PHE | A | 248 | 34.111 | 33.937 | -8.942 | 1.00 | 9.86 | A |
| ATOM | 1111 | CE1 | PHE | A | 248 | 33.853 | 36.076 | -7.186 | 1.00 | 8.69 | A |
| ATOM | 1112 | CE2 | PHE | A | 248 | 33.735 | 33.708 | -7.617 | 1.00 | 9.42 | A |
| ATOM | 1113 | CZ | PHE | A | 248 | 33.607 | 34.781 | -6.738 | 1.00 | 8.27 | A |
| ATOM | 1114 | C | PHE | A | 248 | 37.098 | 34.698 | -10.367 | 1.00 | 8.86 | A |
| ATOM | 1115 | O | PHE | A | 248 | 37.636 | 34.861 | -9.274 | 1.00 | 9.14 | A |
| ATOM | 1116 | N | LEU | A | 249 | 37.205 | 33.567 | -11.059 | 1.00 | 9.66 | A |
| ATOM | 1117 | CA | LEU | A | 249 | 37.971 | 32.435 | -10.542 | 1.00 | 9.31 | A |
| ATOM | 1118 | CB | LEU | A | 249 | 37.736 | 31.195 | -11.415 | 1.00 | 8.82 | A |
| ATOM | 1119 | CG | LEU | A | 249 | 36.283 | 30.708 | -11.405 | 1.00 | 13.09 | A |
| ATOM | 1120 | CD1 | LEU | A | 249 | 36.127 | 29.567 | -12.393 | 1.00 | 13.38 | A |
| ATOM | 1121 | CD2 | LEU | A | 249 | 35.888 | 30.265 | -9.996 | 1.00 | 12.31 | A |
| ATOM | 1122 | C | LEU | A | 249 | 39.462 | 32.744 | -10.429 | 1.00 | 10.28 | A |
| ATOM | 1123 | O | LEU | A | 249 | 40.126 | 32.268 | -9.505 | 1.00 | 9.43 | A |
| ATOM | 1124 | N | ARG | A | 250 | 39.999 | 33.536 | -11.355 | 1.00 | 9.79 | A |
| ATOM | 1125 | CA | ARG | A | 250 | 41.410 | 33.897 | -11.270 | 1.00 | 9.23 | A |
| ATOM | 1126 | CB | ARG | A | 250 | 41.899 | 34.549 | -12.573 | 1.00 | 10.09 | A |
| ATOM | 1127 | CG | ARG | A | 250 | 41.905 | 33.591 | -13.770 | 1.00 | 10.89 | A |
| ATOM | 1128 | CD | ARG | A | 250 | 42.923 | 34.015 | -14.832 | 1.00 | 12.35 | A |
| ATOM | 1129 | NE | ARG | A | 250 | 42.692 | 35.372 | -15.318 | 1.00 | 14.15 | A |
| ATOM | 1130 | CZ | ARG | A | 250 | 41.768 | 35.713 | -16.213 | 1.00 | 12.84 | A |
| ATOM | 1131 | NH1 | ARG | A | 250 | 40.968 | 34.793 | -16.744 | 1.00 | 12.74 | A |
| ATOM | 1132 | NH2 | ARG | A | 250 | 41.642 | 36.985 | -16.573 | 1.00 | 13.32 | A |
| ATOM | 1133 | C | ARG | A | 250 | 41.617 | 34.851 | -10.087 | 1.00 | 9.42 | A |
| ATOM | 1134 | O | ARG | A | 250 | 42.674 | 34.852 | -9.461 | 1.00 | 10.80 | A |
| ATOM | 1135 | N | MSE | A | 251 | 40.603 | 35.660 | -9.786 | 1.00 | 8.99 | A |
| ATOM | 1136 | CA | MSE | A | 251 | 40.693 | 36.585 | -8.664 | 1.00 | 7.90 | A |
| ATOM | 1137 | CB | MSE | A | 251 | 39.503 | 37.546 | -8.655 | 1.00 | 10.28 | A |
| ATOM | 1138 | CG | MSE | A | 251 | 39.546 | 38.555 | -9.787 | 1.00 | 10.58 | A |
| ATOM | 1139 | SE | MSE | A | 251 | 37.927 | 39.597 | -9.882 | 1.00 | 19.52 | A |
| ATOM | 1140 | CE | MSE | A | 251 | 38.253 | 40.781 | -8.392 | 1.00 | 16.71 | A |
| ATOM | 1141 | C | MSE | A | 251 | 40.728 | 35.785 | -7.368 | 1.00 | 8.49 | A |
| ATOM | 1142 | O | MSE | A | 251 | 41.453 | 36.134 | -6.441 | 1.00 | 8.06 | A |
| ATOM | 1143 | N | LEU | A | 252 | 39.946 | 34.708 | -7.306 | 1.00 | 8.09 | A |
| ATOM | 1144 | CA | LEU | A | 252 | 39.936 | 33.873 | -6.109 | 1.00 | 8.04 | A |
| ATOM | 1145 | CB | LEU | A | 252 | 38.891 | 32.757 | -6.222 | 1.00 | 8.32 | A |
| ATOM | 1146 | CG | LEU | A | 252 | 37.411 | 33.159 | -6.168 | 1.00 | 8.66 | A |
| ATOM | 1147 | CD1 | LEU | A | 252 | 36.544 | 31.914 | -6.288 | 1.00 | 9.22 | A |
| ATOM | 1148 | CD2 | LEU | A | 252 | 37.104 | 33.889 | -4.867 | 1.00 | 9.32 | A |
| ATOM | 1149 | C | LEU | A | 252 | 41.314 | 33.262 | -5.899 | 1.00 | 9.42 | A |
| ATOM | 1150 | O | LEU | A | 252 | 41.800 | 33.177 | -4.771 | 1.00 | 9.61 | A |
| ATOM | 1151 | N | LEU | A | 253 | 41.944 | 32.834 | -6.990 | 1.00 | 9.24 | A |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1152 | CA | LEU | A | 253 | 43.271 | 32.239 | -6.910 | 1.00 | 11.62 | A |
| ATOM | 1153 | CB | LEU | A | 253 | 43.696 | 31.706 | -8.282 | 1.00 | 13.39 | A |
| ATOM | 1154 | CG | LEU | A | 253 | 45.049 | 30.990 | -8.331 | 1.00 | 17.43 | A |
| ATOM | 1155 | CD1 | LEU | A | 253 | 45.023 | 29.793 | -7.394 | 1.00 | 20.44 | A |
| ATOM | 1156 | CD2 | LEU | A | 253 | 45.351 | 30.550 | -9.761 | 1.00 | 20.02 | A |
| ATOM | 1157 | C | LEU | A | 253 | 44.276 | 33.279 | -6.413 | 1.00 | 11.13 | A |
| ATOM | 1158 | O | LEU | A | 253 | 45.169 | 32.960 | -5.627 | 1.00 | 11.41 | A |
| ATOM | 1159 | N | ARG | A | 254 | 44.129 | 34.520 | -6.871 | 1.00 | 11.69 | A |
| ATOM | 1160 | CA | ARG | A | 254 | 45.022 | 35.600 | -6.450 | 1.00 | 13.18 | A |
| ATOM | 1161 | CB | ARG | A | 254 | 44.700 | 36.888 | -7.219 | 1.00 | 15.17 | A |
| ATOM | 1162 | CG | ARG | A | 254 | 45.686 | 38.045 | -7.004 | 1.00 | 21.07 | A |
| ATOM | 1163 | CD | ARG | A | 254 | 47.047 | 37.763 | -7.645 | 1.00 | 26.19 | A |
| ATOM | 1164 | NE | ARG | A | 254 | 47.962 | 37.064 | -6.746 | 1.00 | 35.54 | A |
| ATOM | 1165 | CZ | ARG | A | 254 | 48.623 | 37.648 | -5.751 | 1.00 | 38.24 | A |
| ATOM | 1166 | NH1 | ARG | A | 254 | 48.474 | 38.948 | -5.527 | 1.00 | 41.13 | A |
| ATOM | 1167 | NH2 | ARG | A | 254 | 49.434 | 36.934 | -4.979 | 1.00 | 39.76 | A |
| ATOM | 1168 | C | ARG | A | 254 | 44.860 | 35.835 | -4.943 | 1.00 | 12.40 | A |
| ATOM | 1169 | O | ARG | A | 254 | 45.843 | 36.054 | -4.233 | 1.00 | 13.42 | A |
| ATOM | 1170 | N | LEU | A | 255 | 43.623 | 35.788 | -4.452 | 1.00 | 11.26 | A |
| ATOM | 1171 | CA | LEU | A | 255 | 43.383 | 35.977 | -3.023 | 1.00 | 11.62 | A |
| ATOM | 1172 | CB | LEU | A | 255 | 41.879 | 36.014 | -2.717 | 1.00 | 12.84 | A |
| ATOM | 1173 | CG | LEU | A | 255 | 41.140 | 37.298 | -3.105 | 1.00 | 17.32 | A |
| ATOM | 1174 | CD1 | LEU | A | 255 | 39.664 | 37.180 | -2.748 | 1.00 | 15.50 | A |
| ATOM | 1175 | CD2 | LEU | A | 255 | 41.770 | 38.479 | -2.372 | 1.00 | 16.31 | A |
| ATOM | 1176 | C | LEU | A | 255 | 44.043 | 34.852 | -2.226 | 1.00 | 12.01 | A |
| ATOM | 1177 | O | LEU | A | 255 | 44.672 | 35.103 | -1.197 | 1.00 | 10.55 | A |
| ATOM | 1178 | N | ALA | A | 256 | 43.901 | 33.616 | -2.701 | 1.00 | 12.67 | A |
| ATOM | 1179 | CA | ALA | A | 256 | 44.507 | 32.474 | -2.017 | 1.00 | 14.15 | A |
| ATOM | 1180 | CB | ALA | A | 256 | 44.103 | 31.165 | -2.701 | 1.00 | 12.71 | A |
| ATOM | 1181 | C | ALA | A | 256 | 46.029 | 32.614 | -1.996 | 1.00 | 15.50 | A |
| ATOM | 1182 | O | ALA | A | 256 | 46.671 | 32.310 | -.988 | 1.00 | 17.69 | A |
| ATOM | 1183 | N | ASP | A | 257 | 46.601 | 33.077 | -3.106 | 1.00 | 16.20 | A |
| ATOM | 1184 | CA | ASP | A | 257 | 48.050 | 33.266 | -3.209 | 1.00 | 18.87 | A |
| ATOM | 1185 | CB | ASP | A | 257 | 48.465 | 33.654 | -4.633 | 1.00 | 20.67 | A |
| ATOM | 1186 | CG | ASP | A | 257 | 48.336 | 32.520 | -5.621 | 1.00 | 25.45 | A |
| ATOM | 1187 | OD1 | ASP | A | 257 | 48.382 | 31.348 | -5.202 | 1.00 | 26.70 | A |
| ATOM | 1188 | OD2 | ASP | A | 257 | 48.210 | 32.812 | -6.830 | 1.00 | 27.63 | A |
| ATOM | 1189 | C | ASP | A | 257 | 48.536 | 34.380 | -2.296 | 1.00 | 18.97 | A |
| ATOM | 1190 | O | ASP | A | 257 | 49.505 | 34.227 | -1.552 | 1.00 | 19.55 | A |
| ATOM | 1191 | N | GLU | A | 258 | 47.852 | 35.512 | -2.374 | 1.00 | 15.45 | A |
| ATOM | 1192 | CA | GLU | A | 258 | 48.214 | 36.695 | -1.613 | 1.00 | 15.96 | A |
| ATOM | 1193 | CB | GLU | A | 258 | 47.364 | 37.874 | -2.090 | 1.00 | 15.35 | A |
| ATOM | 1194 | CG | GLU | A | 258 | 47.812 | 39.233 | -1.579 | 1.00 | 19.78 | A |
| ATOM | 1195 | CD | GLU | A | 258 | 49.205 | 39.596 | -2.052 | 1.00 | 21.75 | A |
| ATOM | 1196 | OE1 | GLU | A | 258 | 49.551 | 39.254 | -3.204 | 1.00 | 24.81 | A |
| ATOM | 1197 | OE2 | GLU | A | 258 | 49.949 | 40.232 | -1.277 | 1.00 | 24.19 | A |
| ATOM | 1198 | C | GLU | A | 258 | 48.098 | 36.580 | -.100 | 1.00 | 15.06 | A |
| ATOM | 1199 | O | GLU | A | 258 | 49.035 | 36.918 | .627 | 1.00 | 14.21 | A |
| ATOM | 1200 | N | PHE | A | 259 | 46.953 | 36.092 | .365 | 1.00 | 12.81 | A |
| ATOM | 1201 | CA | PHE | A | 259 | 46.678 | 36.003 | 1.794 | 1.00 | 12.40 | A |
| ATOM | 1202 | CB | PHE | A | 259 | 45.275 | 36.549 | 2.048 | 1.00 | 14.06 | A |
| ATOM | 1203 | CG | PHE | A | 259 | 45.103 | 37.973 | 1.612 | 1.00 | 13.57 | A |
| ATOM | 1204 | CD1 | PHE | A | 259 | 45.752 | 39.002 | 2.290 | 1.00 | 15.40 | A |
| ATOM | 1205 | CD2 | PHE | A | 259 | 44.322 | 38.288 | .505 | 1.00 | 13.21 | A |
| ATOM | 1206 | CE1 | PHE | A | 259 | 45.625 | 40.326 | 1.872 | 1.00 | 14.07 | A |
| ATOM | 1207 | CE2 | PHE | A | 259 | 44.188 | 39.610 | .078 | 1.00 | 13.61 | A |
| ATOM | 1208 | CZ | PHE | A | 259 | 44.842 | 40.631 | .763 | 1.00 | 15.29 | A |
| ATOM | 1209 | C | PHE | A | 259 | 46.828 | 34.642 | 2.461 | 1.00 | 13.00 | A |
| ATOM | 1210 | O | PHE | A | 259 | 46.724 | 34.539 | 3.684 | 1.00 | 14.38 | A |
| ATOM | 1211 | N | GLY | A | 260 | 47.068 | 33.604 | 1.668 | 1.00 | 12.99 | A |
| ATOM | 1212 | CA | GLY | A | 260 | 47.242 | 32.276 | 2.227 | 1.00 | 13.13 | A |
| ATOM | 1213 | C | GLY | A | 260 | 45.980 | 31.705 | 2.844 | 1.00 | 14.85 | A |
| ATOM | 1214 | O | GLY | A | 260 | 46.039 | 30.916 | 3.785 | 1.00 | 17.57 | A |
| ATOM | 1215 | N | VAL | A | 261 | 44.832 | 32.120 | 2.330 | 1.00 | 12.38 | A |
| ATOM | 1216 | CA | VAL | A | 261 | 43.568 | 31.615 | 2.843 | 1.00 | 11.17 | A |
| ATOM | 1217 | CB | VAL | A | 261 | 42.446 | 32.672 | 2.766 | 1.00 | 12.70 | A |
| ATOM | 1218 | CG1 | VAL | A | 261 | 42.764 | 33.841 | 3.681 | 1.00 | 13.51 | A |
| ATOM | 1219 | CG2 | VAL | A | 261 | 42.274 | 33.140 | 1.334 | 1.00 | 13.33 | A |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1220 | C | VAL | A | 261 | 43.118 | 30.429 | 2.021 | 1.00 | 10.55 | A |
| ATOM | 1221 | O | VAL | A | 261 | 43.524 | 30.265 | .871 | 1.00 | 11.12 | A |
| ATOM | 1222 | N | ALA | A | 262 | 42.285 | 29.594 | 2.623 | 1.00 | 8.95 | A |
| ATOM | 1223 | CA | ALA | A | 262 | 41.727 | 28.464 | 1.911 | 1.00 | 7.48 | A |
| ATOM | 1224 | CB | ALA | A | 262 | 41.299 | 27.378 | 2.886 | 1.00 | 8.32 | A |
| ATOM | 1225 | C | ALA | A | 262 | 40.508 | 29.059 | 1.224 | 1.00 | 8.31 | A |
| ATOM | 1226 | O | ALA | A | 262 | 39.759 | 29.815 | 1.842 | 1.00 | 11.69 | A |
| ATOM | 1227 | N | VAL | A | 263 | 40.322 | 28.746 | -.053 | 1.00 | 6.91 | A |
| ATOM | 1228 | CA | VAL | A | 263 | 39.160 | 29.236 | -.781 | 1.00 | 8.79 | A |
| ATOM | 1229 | CB | VAL | A | 263 | 39.563 | 29.988 | -2.064 | 1.00 | 6.94 | A |
| ATOM | 1230 | CG1 | VAL | A | 263 | 38.314 | 30.359 | -2.868 | 1.00 | 9.46 | A |
| ATOM | 1231 | CG2 | VAL | A | 263 | 40.349 | 31.238 | -1.698 | 1.00 | 9.49 | A |
| ATOM | 1232 | C | VAL | A | 263 | 38.330 | 28.020 | -1.150 | 1.00 | 7.77 | A |
| ATOM | 1233 | O | VAL | A | 263 | 38.807 | 27.124 | -1.842 | 1.00 | 10.31 | A |
| ATOM | 1234 | N | VAL | A | 264 | 37.094 | 27.984 | -.664 | 1.00 | 8.77 | A |
| ATOM | 1235 | CA | VAL | A | 264 | 36.196 | 26.870 | -.933 | 1.00 | 8.22 | A |
| ATOM | 1236 | CB | VAL | A | 264 | 35.721 | 26.217 | .381 | 1.00 | 8.51 | A |
| ATOM | 1237 | CG1 | VAL | A | 264 | 34.704 | 25.114 | .082 | 1.00 | 10.31 | A |
| ATOM | 1238 | CG2 | VAL | A | 264 | 36.912 | 25.668 | 1.148 | 1.00 | 9.45 | A |
| ATOM | 1239 | C | VAL | A | 264 | 34.984 | 27.389 | -1.686 | 1.00 | 9.72 | A |
| ATOM | 1240 | O | VAL | A | 264 | 34.284 | 28.280 | -1.205 | 1.00 | 11.71 | A |
| ATOM | 1241 | N | ILE | A | 265 | 34.738 | 26.837 | -2.868 | 1.00 | 10.40 | A |
| ATOM | 1242 | CA | ILE | A | 265 | 33.600 | 27.263 | -3.660 | 1.00 | 10.29 | A |
| ATOM | 1243 | CB | ILE | A | 265 | 34.047 | 27.971 | -4.957 | 1.00 | 10.14 | A |
| ATOM | 1244 | CG2 | ILE | A | 265 | 35.016 | 29.101 | -4.621 | 1.00 | 11.21 | A |
| ATOM | 1245 | CG1 | ILE | A | 265 | 34.708 | 26.966 | -5.907 | 1.00 | 12.27 | A |
| ATOM | 1246 | CD1 | ILE | A | 265 | 35.143 | 27.565 | -7.238 | 1.00 | 13.03 | A |
| ATOM | 1247 | C | ILE | A | 265 | 32.748 | 26.063 | -4.034 | 1.00 | 10.17 | A |
| ATOM | 1248 | O | ILE | A | 265 | 33.236 | 24.935 | -4.084 | 1.00 | 9.91 | A |
| ATOM | 1249 | N | THR | A | 266 | 31.470 | 26.305 | -4.282 | 1.00 | 8.88 | A |
| ATOM | 1250 | CA | THR | A | 266 | 30.584 | 25.225 | -4.676 | 1.00 | 9.58 | A |
| ATOM | 1251 | CB | THR | A | 266 | 29.349 | 25.134 | -3.760 | 1.00 | 10.99 | A |
| ATOM | 1252 | OG1 | THR | A | 266 | 28.518 | 26.287 | -3.941 | 1.00 | 12.11 | A |
| ATOM | 1253 | CG2 | THR | A | 266 | 29.785 | 25.052 | -2.301 | 1.00 | 12.65 | A |
| ATOM | 1254 | C | THR | A | 266 | 30.161 | 25.483 | -6.112 | 1.00 | 11.50 | A |
| ATOM | 1255 | O | THR | A | 266 | 30.132 | 26.628 | -6.565 | 1.00 | 12.79 | A |
| ATOM | 1256 | N | ASN | A | 267 | 29.850 | 24.410 | -6.828 | 1.00 | 12.20 | A |
| ATOM | 1257 | CA | ASN | A | 267 | 29.465 | 24.504 | -8.227 | 1.00 | 13.60 | A |
| ATOM | 1258 | CB | ASN | A | 267 | 30.686 | 24.223 | -9.103 | 1.00 | 14.59 | A |
| ATOM | 1259 | CG | ASN | A | 267 | 30.539 | 24.763 | -10.510 | 1.00 | 17.75 | A |
| ATOM | 1260 | OD1 | ASN | A | 267 | 29.429 | 24.953 | -11.008 | 1.00 | 19.43 | A |
| ATOM | 1261 | ND2 | ASN | A | 267 | 31.667 | 25.002 | -11.166 | 1.00 | 17.66 | A |
| ATOM | 1262 | C | ASN | A | 267 | 28.391 | 23.458 | -8.494 | 1.00 | 15.70 | A |
| ATOM | 1263 | O | ASN | A | 267 | 28.267 | 22.495 | -7.738 | 1.00 | 15.21 | A |
| ATOM | 1264 | N | ALA | A | 293 | 40.359 | 24.063 | -14.750 | 1.00 | 25.75 | A |
| ATOM | 1265 | CA | ALA | A | 293 | 40.748 | 24.289 | -13.361 | 1.00 | 26.09 | A |
| ATOM | 1266 | CB | ALA | A | 293 | 40.228 | 23.156 | -12.482 | 1.00 | 26.24 | A |
| ATOM | 1267 | C | ALA | A | 293 | 42.263 | 24.395 | -13.226 | 1.00 | 26.19 | A |
| ATOM | 1268 | O | ALA | A | 293 | 43.008 | 23.745 | -13.960 | 1.00 | 26.65 | A |
| ATOM | 1269 | N | HIS | A | 294 | 42.712 | 25.216 | -12.283 | 1.00 | 24.21 | A |
| ATOM | 1270 | CA | HIS | A | 294 | 44.140 | 25.393 | -12.051 | 1.00 | 23.37 | A |
| ATOM | 1271 | CB | HIS | A | 294 | 44.377 | 26.568 | -11.098 | 1.00 | 23.08 | A |
| ATOM | 1272 | CG | HIS | A | 294 | 45.820 | 26.933 | -10.933 | 1.00 | 25.13 | A |
| ATOM | 1273 | CD2 | HIS | A | 294 | 46.623 | 27.742 | -11.665 | 1.00 | 25.75 | A |
| ATOM | 1274 | ND1 | HIS | A | 294 | 46.605 | 26.429 | -9.919 | 1.00 | 24.49 | A |
| ATOM | 1275 | CE1 | HIS | A | 294 | 47.831 | 26.914 | -10.032 | 1.00 | 26.77 | A |
| ATOM | 1276 | NE2 | HIS | A | 294 | 47.867 | 27.712 | -11.084 | 1.00 | 26.73 | A |
| ATOM | 1277 | C | HIS | A | 294 | 44.713 | 24.110 | -11.463 | 1.00 | 21.69 | A |
| ATOM | 1278 | O | HIS | A | 294 | 43.996 | 23.323 | -10.841 | 1.00 | 20.98 | A |
| ATOM | 1279 | N | ALA | A | 295 | 46.006 | 23.897 | -11.672 | 1.00 | 20.58 | A |
| ATOM | 1280 | CA | ALA | A | 295 | 46.677 | 22.704 | -11.173 | 1.00 | 20.25 | A |
| ATOM | 1281 | CB | ALA | A | 295 | 48.154 | 22.749 | -11.553 | 1.00 | 20.07 | A |
| ATOM | 1282 | C | ALA | A | 295 | 46.534 | 22.525 | -9.662 | 1.00 | 19.38 | A |
| ATOM | 1283 | O | ALA | A | 295 | 46.484 | 21.397 | -9.170 | 1.00 | 20.16 | A |
| ATOM | 1284 | N | SER | A | 296 | 46.451 | 23.632 | -8.930 | 1.00 | 18.12 | A |
| ATOM | 1285 | CA | SER | A | 296 | 46.341 | 23.574 | -7.472 | 1.00 | 17.16 | A |
| ATOM | 1286 | CB | SER | A | 296 | 46.902 | 24.858 | -6.853 | 1.00 | 17.73 | A |
| ATOM | 1287 | OG | SER | A | 296 | 46.143 | 25.993 | -7.244 | 1.00 | 17.47 | A |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1288 | C | SER | A | 296 | 44.929 | 23.347 | -6.943 | 1.00 | 18.00 | A |
| ATOM | 1289 | O | SER | A | 296 | 44.744 | 23.083 | -5.755 | 1.00 | 17.02 | A |
| ATOM | 1290 | N | THR | A | 297 | 43.934 | 23.438 | -7.816 | 1.00 | 15.86 | A |
| ATOM | 1291 | CA | THR | A | 297 | 42.552 | 23.259 | -7.393 | 1.00 | 16.19 | A |
| ATOM | 1292 | CB | THR | A | 297 | 41.580 | 23.837 | -8.446 | 1.00 | 16.61 | A |
| ATOM | 1293 | OG1 | THR | A | 297 | 41.795 | 25.249 | -8.558 | 1.00 | 19.45 | A |
| ATOM | 1294 | CG2 | THR | A | 297 | 40.130 | 23.589 | -8.042 | 1.00 | 18.10 | A |
| ATOM | 1295 | C | THR | A | 297 | 42.186 | 21.804 | -7.121 | 1.00 | 16.88 | A |
| ATOM | 1296 | O | THR | A | 297 | 42.511 | 20.910 | -7.899 | 1.00 | 19.37 | A |
| ATOM | 1297 | N | THR | A | 298 | 41.522 | 21.579 | -5.993 | 1.00 | 14.80 | A |
| ATOM | 1298 | CA | THR | A | 298 | 41.072 | 20.248 | -5.609 | 1.00 | 14.89 | A |
| ATOM | 1299 | CB | THR | A | 298 | 41.282 | 19.988 | -4.103 | 1.00 | 16.40 | A |
| ATOM | 1300 | OG1 | THR | A | 298 | 42.680 | 19.966 | -3.812 | 1.00 | 18.58 | A |
| ATOM | 1301 | CG2 | THR | A | 298 | 40.672 | 18.650 | -3.697 | 1.00 | 18.79 | A |
| ATOM | 1302 | C | THR | A | 298 | 39.581 | 20.203 | -5.890 | 1.00 | 13.32 | A |
| ATOM | 1303 | O | THR | A | 298 | 38.838 | 21.043 | -5.398 | 1.00 | 12.51 | A |
| ATOM | 1304 | N | ARG | A | 299 | 39.149 | 19.232 | -6.688 | 1.00 | 13.14 | A |
| ATOM | 1305 | CA | ARG | A | 299 | 37.735 | 19.094 | -7.007 | 1.00 | 13.42 | A |
| ATOM | 1306 | CB | ARG | A | 299 | 37.543 | 18.923 | -8.513 | 1.00 | 14.70 | A |
| ATOM | 1307 | CG | ARG | A | 299 | 37.595 | 20.223 | -9.282 | 1.00 | 15.90 | A |
| ATOM | 1308 | CD | ARG | A | 299 | 37.341 | 19.992 | -10.756 | 1.00 | 18.69 | A |
| ATOM | 1309 | NE | ARG | A | 299 | 37.088 | 21.244 | -11.455 | 1.00 | 22.79 | A |
| ATOM | 1310 | CZ | ARG | A | 299 | 36.981 | 21.349 | -12.773 | 1.00 | 23.75 | A |
| ATOM | 1311 | NH1 | ARG | A | 299 | 37.111 | 20.271 | -13.535 | 1.00 | 25.24 | A |
| ATOM | 1312 | NH2 | ARG | A | 299 | 36.738 | 22.528 | -13.327 | 1.00 | 24.88 | A |
| ATOM | 1313 | C | ARG | A | 299 | 37.101 | 17.919 | -6.276 | 1.00 | 13.27 | A |
| ATOM | 1314 | O | ARG | A | 299 | 37.580 | 16.785 | -6.365 | 1.00 | 16.01 | A |
| ATOM | 1315 | N | LEU | A | 300 | 36.024 | 18.201 | -5.550 | 1.00 | 11.42 | A |
| ATOM | 1316 | CA | LEU | A | 300 | 35.302 | 17.181 | -4.799 | 1.00 | 12.66 | A |
| ATOM | 1317 | CB | LEU | A | 300 | 35.158 | 17.594 | -3.333 | 1.00 | 14.16 | A |
| ATOM | 1318 | CG | LEU | A | 300 | 36.415 | 18.043 | -2.589 | 1.00 | 15.24 | A |
| ATOM | 1319 | CD1 | LEU | A | 300 | 36.058 | 18.364 | -1.142 | 1.00 | 15.73 | A |
| ATOM | 1320 | CD2 | LEU | A | 300 | 37.469 | 16.963 | -2.654 | 1.00 | 17.90 | A |
| ATOM | 1321 | C | LEU | A | 300 | 33.913 | 17.004 | -5.391 | 1.00 | 13.73 | A |
| ATOM | 1322 | O | LEU | A | 300 | 33.200 | 17.981 | -5.615 | 1.00 | 14.00 | A |
| ATOM | 1323 | N | TYR | A | 301 | 33.531 | 15.756 | -5.649 | 1.00 | 13.54 | A |
| ATOM | 1324 | CA | TYR | A | 301 | 32.213 | 15.463 | -6.197 | 1.00 | 13.49 | A |
| ATOM | 1325 | CB | TYR | A | 301 | 32.336 | 14.587 | -7.446 | 1.00 | 15.65 | A |
| ATOM | 1326 | CG | TYR | A | 301 | 33.051 | 15.291 | -8.577 | 1.00 | 17.58 | A |
| ATOM | 1327 | CD1 | TYR | A | 301 | 34.443 | 15.368 | -8.606 | 1.00 | 18.47 | A |
| ATOM | 1328 | CE1 | TYR | A | 301 | 35.105 | 16.079 | -9.602 | 1.00 | 19.95 | A |
| ATOM | 1329 | CD2 | TYR | A | 301 | 32.332 | 15.945 | -9.581 | 1.00 | 18.30 | A |
| ATOM | 1330 | CE2 | TYR | A | 301 | 32.985 | 16.661 | -10.583 | 1.00 | 20.78 | A |
| ATOM | 1331 | CZ | TYR | A | 301 | 34.371 | 16.725 | -10.584 | 1.00 | 21.42 | A |
| ATOM | 1332 | OH | TYR | A | 301 | 35.025 | 17.440 | -11.563 | 1.00 | 24.94 | A |
| ATOM | 1333 | C | TYR | A | 301 | 31.390 | 14.768 | -5.122 | 1.00 | 13.26 | A |
| ATOM | 1334 | O | TYR | A | 301 | 31.678 | 13.634 | -4.741 | 1.00 | 14.37 | A |
| ATOM | 1335 | N | LEU | A | 302 | 30.369 | 15.465 | -4.633 | 1.00 | 11.70 | A |
| ATOM | 1336 | CA | LEU | A | 302 | 29.518 | 14.945 | -3.570 | 1.00 | 12.66 | A |
| ATOM | 1337 | CB | LEU | A | 302 | 29.176 | 16.067 | -2.584 | 1.00 | 13.35 | A |
| ATOM | 1338 | CG | LEU | A | 302 | 30.341 | 16.918 | -2.075 | 1.00 | 14.08 | A |
| ATOM | 1339 | CD1 | LEU | A | 302 | 29.806 | 18.031 | -1.184 | 1.00 | 16.90 | A |
| ATOM | 1340 | CD2 | LEU | A | 302 | 31.327 | 16.046 | -1.317 | 1.00 | 14.36 | A |
| ATOM | 1341 | C | LEU | A | 302 | 28.221 | 14.332 | -4.081 | 1.00 | 14.19 | A |
| ATOM | 1342 | O | LEU | A | 302 | 27.629 | 14.816 | -5.046 | 1.00 | 15.47 | A |
| ATOM | 1343 | N | ARG | A | 303 | 27.783 | 13.264 | -3.427 | 1.00 | 14.19 | A |
| ATOM | 1344 | CA | ARG | A | 303 | 26.531 | 12.624 | -3.796 | 1.00 | 16.12 | A |
| ATOM | 1345 | CB | ARG | A | 303 | 26.757 | 11.496 | -4.807 | 1.00 | 16.82 | A |
| ATOM | 1346 | CG | ARG | A | 303 | 27.559 | 10.303 | -4.318 | 1.00 | 18.49 | A |
| ATOM | 1347 | CD | ARG | A | 303 | 27.532 | 9.215 | -5.390 | 1.00 | 20.58 | A |
| ATOM | 1348 | NE | ARG | A | 303 | 28.155 | 7.963 | -4.968 | 1.00 | 22.33 | A |
| ATOM | 1349 | CZ | ARG | A | 303 | 29.466 | 7.745 | -4.928 | 1.00 | 24.00 | A |
| ATOM | 1350 | NH1 | ARG | A | 303 | 30.318 | 8.698 | -5.286 | 1.00 | 24.08 | A |
| ATOM | 1351 | NH2 | ARG | A | 303 | 29.926 | 6.561 | -4.541 | 1.00 | 24.43 | A |
| ATOM | 1352 | C | ARG | A | 303 | 25.846 | 12.099 | -2.543 | 1.00 | 17.08 | A |
| ATOM | 1353 | O | ARG | A | 303 | 26.469 | 11.966 | -1.485 | 1.00 | 15.73 | A |
| ATOM | 1354 | N | LYS | A | 304 | 24.556 | 11.810 | -2.659 | 1.00 | 16.79 | A |
| ATOM | 1355 | CA | LYS | A | 304 | 23.812 | 11.334 | -1.511 | 1.00 | 17.94 | A |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1356 | CB | LYS | A | 304 | 22.314 | 11.601 | -1.690 | 1.00 | 18.58 | A |
| ATOM | 1357 | CG | LYS | A | 304 | 21.506 | 11.138 | -.488 | 1.00 | 22.70 | A |
| ATOM | 1358 | CD | LYS | A | 304 | 20.282 | 11.987 | -.235 | 1.00 | 24.03 | A |
| ATOM | 1359 | CE | LYS | A | 304 | 19.806 | 11.807 | 1.199 | 1.00 | 21.77 | A |
| ATOM | 1360 | NZ | LYS | A | 304 | 19.638 | 10.368 | 1.563 | 1.00 | 19.38 | A |
| ATOM | 1361 | C | LYS | A | 304 | 24.025 | 9.868 | -1.172 | 1.00 | 16.85 | A |
| ATOM | 1362 | O | LYS | A | 304 | 24.151 | 9.015 | -2.055 | 1.00 | 18.41 | A |
| ATOM | 1363 | N | GLY | A | 305 | 24.089 | 9.604 | .128 | 1.00 | 16.74 | A |
| ATOM | 1364 | CA | GLY | A | 305 | 24.237 | 8.254 | .637 | 1.00 | 16.44 | A |
| ATOM | 1365 | C | GLY | A | 305 | 22.957 | 7.994 | 1.404 | 1.00 | 16.49 | A |
| ATOM | 1366 | O | GLY | A | 305 | 22.066 | 8.843 | 1.414 | 1.00 | 16.52 | A |
| ATOM | 1367 | N | ARG | A | 306 | 22.838 | 6.844 | 2.057 | 1.00 | 17.03 | A |
| ATOM | 1368 | CA | ARG | A | 306 | 21.614 | 6.569 | 2.798 | 1.00 | 18.22 | A |
| ATOM | 1369 | CB | ARG | A | 306 | 21.575 | 5.110 | 3.261 | 1.00 | 21.45 | A |
| ATOM | 1370 | CG | ARG | A | 306 | 20.253 | 4.741 | 3.913 | 1.00 | 27.33 | A |
| ATOM | 1371 | CD | ARG | A | 306 | 20.090 | 3.243 | 4.113 | 1.00 | 32.41 | A |
| ATOM | 1372 | NE | ARG | A | 306 | 21.051 | 2.699 | 5.067 | 1.00 | 36.11 | A |
| ATOM | 1373 | CZ | ARG | A | 306 | 20.914 | 1.520 | 5.662 | 1.00 | 37.74 | A |
| ATOM | 1374 | NH1 | ARG | A | 306 | 19.853 | .768 | 5.399 | 1.00 | 39.22 | A |
| ATOM | 1375 | NH2 | ARG | A | 306 | 21.831 | 1.092 | 6.520 | 1.00 | 39.30 | A |
| ATOM | 1376 | C | ARG | A | 306 | 21.448 | 7.493 | 4.002 | 1.00 | 16.95 | A |
| ATOM | 1377 | O | ARG | A | 306 | 22.409 | 7.795 | 4.710 | 1.00 | 16.27 | A |
| ATOM | 1378 | N | GLY | A | 307 | 20.220 | 7.954 | 4.221 | 1.00 | 16.74 | A |
| ATOM | 1379 | CA | GLY | A | 307 | 19.946 | 8.824 | 5.350 | 1.00 | 14.78 | A |
| ATOM | 1380 | C | GLY | A | 307 | 20.798 | 10.080 | 5.393 | 1.00 | 16.48 | A |
| ATOM | 1381 | O | GLY | A | 307 | 20.848 | 10.843 | 4.426 | 1.00 | 15.11 | A |
| ATOM | 1382 | N | GLU | A | 308 | 21.476 | 10.289 | 6.519 | 1.00 | 16.48 | A |
| ATOM | 1383 | CA | GLU | A | 308 | 22.318 | 11.467 | 6.694 | 1.00 | 17.56 | A |
| ATOM | 1384 | CB | GLU | A | 308 | 22.399 | 11.838 | 8.182 | 1.00 | 19.01 | A |
| ATOM | 1385 | CG | GLU | A | 308 | 23.297 | 10.947 | 9.053 | 1.00 | 21.25 | A |
| ATOM | 1386 | CD | GLU | A | 308 | 22.828 | 9.501 | 9.145 | 1.00 | 24.06 | A |
| ATOM | 1387 | OE1 | GLU | A | 308 | 21.610 | 9.266 | 9.285 | 1.00 | 23.79 | A |
| ATOM | 1388 | OE2 | GLU | A | 308 | 23.686 | 8.595 | 9.095 | 1.00 | 26.02 | A |
| ATOM | 1389 | C | GLU | A | 308 | 23.726 | 11.301 | 6.132 | 1.00 | 16.66 | A |
| ATOM | 1390 | O | GLU | A | 308 | 24.532 | 12.235 | 6.185 | 1.00 | 15.98 | A |
| ATOM | 1391 | N | THR | A | 309 | 24.032 | 10.127 | 5.586 | 1.00 | 14.19 | A |
| ATOM | 1392 | CA | THR | A | 309 | 25.367 | 9.899 | 5.044 | 1.00 | 15.36 | A |
| ATOM | 1393 | CB | THR | A | 309 | 25.741 | 8.396 | 5.038 | 1.00 | 16.75 | A |
| ATOM | 1394 | OG1 | THR | A | 309 | 24.944 | 7.694 | 4.077 | 1.00 | 17.63 | A |
| ATOM | 1395 | CG2 | THR | A | 309 | 25.515 | 7.794 | 6.416 | 1.00 | 17.50 | A |
| ATOM | 1396 | C | THR | A | 309 | 25.507 | 10.461 | 3.637 | 1.00 | 14.74 | A |
| ATOM | 1397 | O | THR | A | 309 | 24.535 | 10.565 | 2.886 | 1.00 | 14.98 | A |
| ATOM | 1398 | N | ARG | A | 310 | 26.730 | 10.843 | 3.296 | 1.00 | 14.85 | A |
| ATOM | 1399 | CA | ARG | A | 310 | 27.027 | 11.410 | 1.989 | 1.00 | 14.16 | A |
| ATOM | 1400 | CB | ARG | A | 310 | 27.110 | 12.938 | 2.092 | 1.00 | 13.55 | A |
| ATOM | 1401 | CG | ARG | A | 310 | 25.824 | 13.620 | 2.565 | 1.00 | 14.48 | A |
| ATOM | 1402 | CD | ARG | A | 310 | 24.745 | 13.562 | 1.493 | 1.00 | 14.76 | A |
| ATOM | 1403 | NE | ARG | A | 310 | 23.552 | 14.340 | 1.830 | 1.00 | 15.70 | A |
| ATOM | 1404 | CZ | ARG | A | 310 | 22.574 | 13.926 | 2.632 | 1.00 | 16.49 | A |
| ATOM | 1405 | NH1 | ARG | A | 310 | 22.634 | 12.730 | 3.199 | 1.00 | 14.99 | A |
| ATOM | 1406 | NH2 | ARG | A | 310 | 21.523 | 14.708 | 2.854 | 1.00 | 15.34 | A |
| ATOM | 1407 | C | ARG | A | 310 | 28.362 | 10.846 | 1.532 | 1.00 | 13.62 | A |
| ATOM | 1408 | O | ARG | A | 310 | 29.150 | 10.355 | 2.343 | 1.00 | 14.37 | A |
| ATOM | 1409 | N | ILE | A | 311 | 28.619 | 10.911 | .234 | 1.00 | 13.83 | A |
| ATOM | 1410 | CA | ILE | A | 311 | 29.871 | 10.404 | -.297 | 1.00 | 15.05 | A |
| ATOM | 1411 | CB | ILE | A | 311 | 29.633 | 9.181 | -1.206 | 1.00 | 17.49 | A |
| ATOM | 1412 | CG2 | ILE | A | 311 | 30.958 | 8.671 | -1.751 | 1.00 | 19.53 | A |
| ATOM | 1413 | CG1 | ILE | A | 311 | 28.929 | 8.079 | -.412 | 1.00 | 21.16 | A |
| ATOM | 1414 | CD1 | ILE | A | 311 | 28.447 | 6.931 | -1.269 | 1.00 | 24.48 | A |
| ATOM | 1415 | C | ILE | A | 311 | 30.599 | 11.477 | -1.095 | 1.00 | 14.37 | A |
| ATOM | 1416 | O | ILE | A | 311 | 29.989 | 12.222 | -1.866 | 1.00 | 14.03 | A |
| ATOM | 1417 | N | CYS | A | 312 | 31.907 | 11.560 | -.884 | 1.00 | 13.85 | A |
| ATOM | 1418 | CA | CYS | A | 312 | 32.741 | 12.519 | -1.588 | 1.00 | 13.35 | A |
| ATOM | 1419 | CB | CYS | A | 312 | 33.516 | 13.393 | -.597 | 1.00 | 13.04 | A |
| ATOM | 1420 | SG | CYS | A | 312 | 34.710 | 14.505 | -1.391 | 1.00 | 16.96 | A |
| ATOM | 1421 | C | CYS | A | 312 | 33.718 | 11.728 | -2.440 | 1.00 | 14.32 | A |
| ATOM | 1422 | O | CYS | A | 312 | 34.361 | 10.793 | -1.956 | 1.00 | 14.42 | A |
| ATOM | 1423 | N | LYS | A | 313 | 33.825 | 12.097 | -3.710 | 1.00 | 14.16 | A |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1424 | CA | LYS | A | 313 | 34.733 | 11.408 | -4.610 | 1.00 | 15.69 | A |
| ATOM | 1425 | CB | LYS | A | 313 | 33.940 | 10.672 | -5.693 | 1.00 | 18.29 | A |
| ATOM | 1426 | CG | LYS | A | 313 | 34.806 | 9.870 | -6.650 | 1.00 | 21.66 | A |
| ATOM | 1427 | CD | LYS | A | 313 | 33.953 | 9.085 | -7.636 | 1.00 | 27.84 | A |
| ATOM | 1428 | CE | LYS | A | 313 | 34.818 | 8.203 | -8.525 | 1.00 | 31.20 | A |
| ATOM | 1429 | NZ | LYS | A | 313 | 34.006 | 7.412 | -9.494 | 1.00 | 36.03 | A |
| ATOM | 1430 | C | LYS | A | 313 | 35.692 | 12.396 | -5.258 | 1.00 | 16.66 | A |
| ATOM | 1431 | O | LYS | A | 313 | 35.300 | 13.510 | -5.610 | 1.00 | 15.05 | A |
| ATOM | 1432 | N | ILE | A | 314 | 36.950 | 11.985 | -5.391 | 1.00 | 17.72 | A |
| ATOM | 1433 | CA | ILE | A | 314 | 37.977 | 12.812 | -6.016 | 1.00 | 22.21 | A |
| ATOM | 1434 | CB | ILE | A | 314 | 39.083 | 13.192 | -5.016 | 1.00 | 22.48 | A |
| ATOM | 1435 | CG2 | ILE | A | 314 | 40.135 | 14.053 | -5.708 | 1.00 | 26.30 | A |
| ATOM | 1436 | CG1 | ILE | A | 314 | 38.472 | 13.959 | -3.843 | 1.00 | 21.65 | A |
| ATOM | 1437 | CD1 | ILE | A | 314 | 39.476 | 14.366 | -2.786 | 1.00 | 26.01 | A |
| ATOM | 1438 | C | ILE | A | 314 | 38.580 | 12.015 | -7.169 | 1.00 | 26.09 | A |
| ATOM | 1439 | O | ILE | A | 314 | 38.628 | 10.785 | -7.119 | 1.00 | 24.64 | A |
| ATOM | 1440 | N | TYR | A | 315 | 39.047 | 12.718 | -8.197 | 1.00 | 31.43 | A |
| ATOM | 1441 | CA | TYR | A | 315 | 39.607 | 12.073 | -9.383 | 1.00 | 37.29 | A |
| ATOM | 1442 | CB | TYR | A | 315 | 38.827 | 12.518 | -10.616 | 1.00 | 37.68 | A |
| ATOM | 1443 | CG | TYR | A | 315 | 37.426 | 11.976 | -10.689 | 1.00 | 38.88 | A |
| ATOM | 1444 | CD1 | TYR | A | 315 | 37.179 | 10.702 | -11.197 | 1.00 | 39.92 | A |
| ATOM | 1445 | CE1 | TYR | A | 315 | 35.887 | 10.198 | -11.275 | 1.00 | 39.85 | A |
| ATOM | 1446 | CD2 | TYR | A | 315 | 36.342 | 12.736 | -10.255 | 1.00 | 39.19 | A |
| ATOM | 1447 | CE2 | TYR | A | 315 | 35.046 | 12.242 | -10.325 | 1.00 | 39.96 | A |
| ATOM | 1448 | CZ | TYR | A | 315 | 34.825 | 10.971 | -10.839 | 1.00 | 40.03 | A |
| ATOM | 1449 | OH | TYR | A | 315 | 33.547 | 10.474 | -10.922 | 1.00 | 41.58 | A |
| ATOM | 1450 | C | TYR | A | 315 | 41.089 | 12.288 | -9.656 | 1.00 | 41.54 | A |
| ATOM | 1451 | O | TYR | A | 315 | 41.827 | 12.818 | -8.823 | 1.00 | 42.77 | A |
| ATOM | 1452 | N | ASP | A | 316 | 41.488 | 11.867 | -10.857 | 1.00 | 45.11 | A |
| ATOM | 1453 | CA | ASP | A | 316 | 42.856 | 11.955 | -11.364 | 1.00 | 48.76 | A |
| ATOM | 1454 | CB | ASP | A | 316 | 42.913 | 12.906 | -12.562 | 1.00 | 51.10 | A |
| ATOM | 1455 | CG | ASP | A | 316 | 41.986 | 12.483 | -13.685 | 1.00 | 53.20 | A |
| ATOM | 1456 | OD1 | ASP | A | 316 | 41.864 | 11.263 | -13.929 | 1.00 | 54.29 | A |
| ATOM | 1457 | OD2 | ASP | A | 316 | 41.387 | 13.369 | -14.331 | 1.00 | 55.12 | A |
| ATOM | 1458 | C | ASP | A | 316 | 43.901 | 12.364 | -10.339 | 1.00 | 50.29 | A |
| ATOM | 1459 | O | ASP | A | 316 | 44.235 | 13.541 | -10.202 | 1.00 | 50.40 | A |
| ATOM | 1460 | N | SER | A | 317 | 44.419 | 11.370 | -9.628 | 1.00 | 51.63 | A |
| ATOM | 1461 | CA | SER | A | 317 | 45.433 | 11.596 | -8.611 | 1.00 | 53.06 | A |
| ATOM | 1462 | CB | SER | A | 317 | 44.829 | 11.406 | -7.217 | 1.00 | 53.24 | A |
| ATOM | 1463 | OG | SER | A | 317 | 43.646 | 12.170 | -7.060 | 1.00 | 53.77 | A |
| ATOM | 1464 | C | SER | A | 317 | 46.563 | 10.596 | -8.817 | 1.00 | 53.83 | A |
| ATOM | 1465 | O | SER | A | 317 | 46.346 | 9.385 | -8.752 | 1.00 | 54.39 | A |
| ATOM | 1466 | N | PRO | A | 318 | 47.786 | 11.088 | -9.079 | 1.00 | 54.06 | A |
| ATOM | 1467 | CD | PRO | A | 318 | 48.160 | 12.498 | -9.289 | 1.00 | 54.37 | A |
| ATOM | 1468 | CA | PRO | A | 318 | 48.940 | 10.210 | -9.291 | 1.00 | 53.91 | A |
| ATOM | 1469 | CB | PRO | A | 318 | 50.110 | 11.185 | -9.282 | 1.00 | 54.17 | A |
| ATOM | 1470 | CG | PRO | A | 318 | 49.520 | 12.377 | -9.956 | 1.00 | 54.74 | A |
| ATOM | 1471 | C | PRO | A | 318 | 49.057 | 9.138 | -8.213 | 1.00 | 53.87 | A |
| ATOM | 1472 | O | PRO | A | 318 | 49.799 | 8.167 | -8.365 | 1.00 | 54.39 | A |
| ATOM | 1473 | N | CYS | A | 319 | 48.320 | 9.321 | -7.123 | 1.00 | 53.04 | A |
| ATOM | 1474 | CA | CYS | A | 319 | 48.323 | 8.365 | -6.025 | 1.00 | 52.44 | A |
| ATOM | 1475 | CB | CYS | A | 319 | 48.105 | 9.089 | -4.694 | 1.00 | 52.58 | A |
| ATOM | 1476 | SG | CYS | A | 319 | 49.423 | 10.257 | -4.264 | 1.00 | 52.30 | A |
| ATOM | 1477 | C | CYS | A | 319 | 47.226 | 7.326 | -6.247 | 1.00 | 52.16 | A |
| ATOM | 1478 | O | CYS | A | 319 | 47.417 | 6.143 | -5.975 | 1.00 | 52.41 | A |
| ATOM | 1479 | N | LEU | A | 320 | 46.079 | 7.776 | -6.749 | 1.00 | 51.37 | A |
| ATOM | 1480 | CA | LEU | A | 320 | 44.950 | 6.890 | -7.020 | 1.00 | 50.25 | A |
| ATOM | 1481 | CB | LEU | A | 320 | 44.162 | 6.617 | -5.735 | 1.00 | 51.58 | A |
| ATOM | 1482 | CG | LEU | A | 320 | 44.850 | 5.852 | -4.600 | 1.00 | 52.61 | A |
| ATOM | 1483 | CD1 | LEU | A | 320 | 43.919 | 5.791 | -3.401 | 1.00 | 53.53 | A |
| ATOM | 1484 | CD2 | LEU | A | 320 | 45.219 | 4.449 | -5.062 | 1.00 | 53.34 | A |
| ATOM | 1485 | C | LEU | A | 320 | 44.024 | 7.519 | -8.057 | 1.00 | 48.37 | A |
| ATOM | 1486 | O | LEU | A | 320 | 43.617 | 8.673 | -7.917 | 1.00 | 48.51 | A |
| ATOM | 1487 | N | PRO | A | 321 | 43.681 | 6.769 | -9.117 | 1.00 | 46.71 | A |
| ATOM | 1488 | CD | PRO | A | 321 | 44.099 | 5.390 | -9.425 | 1.00 | 46.46 | A |
| ATOM | 1489 | CA | PRO | A | 321 | 42.795 | 7.290 | -10.162 | 1.00 | 44.43 | A |
| ATOM | 1490 | CB | PRO | A | 321 | 42.474 | 6.047 | -10.984 | 1.00 | 45.46 | A |
| ATOM | 1491 | CG | PRO | A | 321 | 43.749 | 5.270 | -10.895 | 1.00 | 46.59 | A |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1492 | C | PRO | A | 321 | 41.545 | 7.927 | -9.562 | 1.00 | 41.95 | A |
| ATOM | 1493 | O | PRO | A | 321 | 41.167 | 9.042 | -9.924 | 1.00 | 40.86 | A |
| ATOM | 1494 | N | GLU | A | 322 | 40.911 | 7.205 | -8.644 | 1.00 | 39.09 | A |
| ATOM | 1495 | CA | GLU | A | 322 | 39.708 | 7.686 | -7.978 | 1.00 | 36.24 | A |
| ATOM | 1496 | CB | GLU | A | 322 | 38.455 | 7.113 | -8.646 | 1.00 | 39.05 | A |
| ATOM | 1497 | CG | GLU | A | 322 | 38.497 | 7.091 | -10.165 | 1.00 | 43.79 | A |
| ATOM | 1498 | CD | GLU | A | 322 | 37.226 | 6.524 | -10.770 | 1.00 | 46.15 | A |
| ATOM | 1499 | OE1 | GLU | A | 322 | 36.680 | 5.555 | -10.200 | 1.00 | 47.26 | A |
| ATOM | 1500 | OE2 | GLU | A | 322 | 36.779 | 7.036 | -11.818 | 1.00 | 48.33 | A |
| ATOM | 1501 | C | GLU | A | 322 | 39.744 | 7.232 | -6.526 | 1.00 | 32.58 | A |
| ATOM | 1502 | O | GLU | A | 322 | 40.264 | 6.161 | -6.213 | 1.00 | 31.65 | A |
| ATOM | 1503 | N | ALA | A | 323 | 39.197 | 8.054 | -5.641 | 1.00 | 26.73 | A |
| ATOM | 1504 | CA | ALA | A | 323 | 39.151 | 7.722 | -4.227 | 1.00 | 23.49 | A |
| ATOM | 1505 | CB | ALA | A | 323 | 40.367 | 8.285 | -3.509 | 1.00 | 24.09 | A |
| ATOM | 1506 | C | ALA | A | 323 | 37.874 | 8.311 | -3.655 | 1.00 | 21.23 | A |
| ATOM | 1507 | O | ALA | A | 323 | 37.432 | 9.382 | -4.074 | 1.00 | 18.44 | A |
| ATOM | 1508 | N | GLU | A | 324 | 37.274 | 7.606 | -2.706 | 1.00 | 20.46 | A |
| ATOM | 1509 | CA | GLU | A | 324 | 36.043 | 8.077 | -2.100 | 1.00 | 21.25 | A |
| ATOM | 1510 | CB | GLU | A | 324 | 34.849 | 7.280 | -2.624 | 1.00 | 23.33 | A |
| ATOM | 1511 | CG | GLU | A | 324 | 34.651 | 7.327 | -4.124 | 1.00 | 27.34 | A |
| ATOM | 1512 | CD | GLU | A | 324 | 33.426 | 6.543 | -4.550 | 1.00 | 29.02 | A |
| ATOM | 1513 | OE1 | GLU | A | 324 | 33.318 | 5.362 | -4.158 | 1.00 | 31.71 | A |
| ATOM | 1514 | OE2 | GLU | A | 324 | 32.576 | 7.101 | -5.272 | 1.00 | 30.39 | A |
| ATOM | 1515 | C | GLU | A | 324 | 36.074 | 7.951 | -.589 | 1.00 | 20.52 | A |
| ATOM | 1516 | O | GLU | A | 324 | 36.831 | 7.158 | -.029 | 1.00 | 21.51 | A |
| ATOM | 1517 | N | ALA | A | 325 | 35.237 | 8.746 | .061 | 1.00 | 18.38 | A |
| ATOM | 1518 | CA | ALA | A | 325 | 35.120 | 8.719 | 1.505 | 1.00 | 18.27 | A |
| ATOM | 1519 | CB | ALA | A | 325 | 36.072 | 9.727 | 2.140 | 1.00 | 18.87 | A |
| ATOM | 1520 | C | ALA | A | 325 | 33.684 | 9.064 | 1.855 | 1.00 | 17.32 | A |
| ATOM | 1521 | O | ALA | A | 325 | 33.044 | 9.869 | 1.178 | 1.00 | 16.37 | A |
| ATOM | 1522 | N | MSE | | 326 | 33.175 | 8.440 | 2.910 | .51 | 16.14 | AC1 |
| ATOM | 1523 | CA | MSE | | 326 | 31.814 | 8.690 | 3.353 | .51 | 15.49 | AC1 |
| ATOM | 1524 | CB | MSE | | 326 | 31.127 | 7.370 | 3.722 | .51 | 16.90 | AC1 |
| ATOM | 1525 | CG | MSE | | 326 | 29.621 | 7.477 | 3.913 | .51 | 17.28 | AC1 |
| ATOM | 1526 | SE | MSE | | 326 | 28.788 | 5.774 | 4.333 | .51 | 21.71 | AC1 |
| ATOM | 1527 | CE | MSE | | 326 | 29.498 | 4.732 | 2.874 | .51 | 24.72 | AC1 |
| ATOM | 1528 | C | MSE | | 326 | 31.863 | 9.603 | 4.571 | .51 | 15.12 | AC1 |
| ATOM | 1529 | O | MSE | | 326 | 32.823 | 9.569 | 5.341 | .51 | 16.04 | AC1 |
| ATOM | 1530 | N | PHE | A | 327 | 30.837 | 10.432 | 4.728 | 1.00 | 14.66 | A |
| ATOM | 1531 | CA | PHE | A | 327 | 30.746 | 11.333 | 5.859 | 1.00 | 13.34 | A |
| ATOM | 1532 | CB | PHE | A | 327 | 31.439 | 12.686 | 5.582 | 1.00 | 14.23 | A |
| ATOM | 1533 | CG | PHE | A | 327 | 30.856 | 13.476 | 4.437 | 1.00 | 12.58 | A |
| ATOM | 1534 | CD1 | PHE | A | 327 | 31.180 | 13.169 | 3.119 | 1.00 | 13.45 | A |
| ATOM | 1535 | CD2 | PHE | A | 327 | 30.024 | 14.568 | 4.685 | 1.00 | 14.05 | A |
| ATOM | 1536 | CE1 | PHE | A | 327 | 30.689 | 13.942 | 2.060 | 1.00 | 13.50 | A |
| ATOM | 1537 | CE2 | PHE | A | 327 | 29.527 | 15.347 | 3.638 | 1.00 | 13.64 | A |
| ATOM | 1538 | CZ | PHE | A | 327 | 29.863 | 15.033 | 2.321 | 1.00 | 13.36 | A |
| ATOM | 1539 | C | PHE | A | 327 | 29.267 | 11.509 | 6.158 | 1.00 | 13.91 | A |
| ATOM | 1540 | O | PHE | A | 327 | 28.416 | 10.945 | 5.466 | 1.00 | 13.73 | A |
| ATOM | 1541 | N | ALA | A | 328 | 28.952 | 12.254 | 7.205 | 1.00 | 13.81 | A |
| ATOM | 1542 | CA | ALA | A | 328 | 27.560 | 12.464 | 7.558 | 1.00 | 13.68 | A |
| ATOM | 1543 | CB | ALA | A | 328 | 27.187 | 11.586 | 8.744 | 1.00 | 15.04 | A |
| ATOM | 1544 | C | ALA | A | 328 | 27.306 | 13.919 | 7.893 | 1.00 | 14.38 | A |
| ATOM | 1545 | O | ALA | A | 328 | 28.210 | 14.631 | 8.326 | 1.00 | 14.71 | A |
| ATOM | 1546 | N | ILE | A | 329 | 26.077 | 14.365 | 7.668 | 1.00 | 14.86 | A |
| ATOM | 1547 | CA | ILE | A | 329 | 25.715 | 15.732 | 7.995 | 1.00 | 16.92 | A |
| ATOM | 1548 | CB | ILE | A | 329 | 25.036 | 16.451 | 6.798 | 1.00 | 18.22 | A |
| ATOM | 1549 | CG2 | ILE | A | 329 | 25.997 | 16.493 | 5.619 | 1.00 | 17.39 | A |
| ATOM | 1550 | CG1 | ILE | A | 329 | 23.752 | 15.733 | 6.383 | 1.00 | 21.82 | A |
| ATOM | 1551 | CD1 | ILE | A | 329 | 23.055 | 16.386 | 5.193 | 1.00 | 25.55 | A |
| ATOM | 1552 | C | ILE | A | 329 | 24.784 | 15.663 | 9.201 | 1.00 | 17.32 | A |
| ATOM | 1553 | O | ILE | A | 329 | 23.758 | 14.979 | 9.179 | 1.00 | 18.02 | A |
| ATOM | 1554 | N | ASN | A | 330 | 25.170 | 16.349 | 10.268 | 1.00 | 17.70 | A |
| ATOM | 1555 | CA | ASN | A | 330 | 24.391 | 16.352 | 11.497 | 1.00 | 18.00 | A |
| ATOM | 1556 | CB | ASN | A | 330 | 25.208 | 15.731 | 12.637 | 1.00 | 20.36 | A |
| ATOM | 1557 | CG | ASN | A | 330 | 25.759 | 14.353 | 12.289 | 1.00 | 21.76 | A |
| ATOM | 1558 | OD1 | ASN | A | 330 | 25.006 | 13.418 | 12.006 | 1.00 | 22.43 | A |
| ATOM | 1559 | ND2 | ASN | A | 330 | 27.081 | 14.223 | 12.314 | 1.00 | 23.90 | A |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1560 | C | ASN | A | 330 | 23.979 | 17.767 | 11.883 | 1.00 | 18.09 | A |
| ATOM | 1561 | O | ASN | A | 330 | 24.365 | 18.743 | 11.235 | 1.00 | 16.82 | A |
| ATOM | 1562 | N | ALA | A | 331 | 23.195 | 17.868 | 12.951 | 1.00 | 18.79 | A |
| ATOM | 1563 | CA | ALA | A | 331 | 22.727 | 19.156 | 13.441 | 1.00 | 19.16 | A |
| ATOM | 1564 | CB | ALA | A | 331 | 21.802 | 18.955 | 14.634 | 1.00 | 20.84 | A |
| ATOM | 1565 | C | ALA | A | 331 | 23.901 | 20.037 | 13.837 | 1.00 | 18.41 | A |
| ATOM | 1566 | O | ALA | A | 331 | 23.822 | 21.261 | 13.740 | 1.00 | 19.60 | A |
| ATOM | 1567 | N | ASP | A | 332 | 24.989 | 19.416 | 14.288 | 1.00 | 18.22 | A |
| ATOM | 1568 | CA | ASP | A | 332 | 26.168 | 20.170 | 14.688 | 1.00 | 17.37 | A |
| ATOM | 1569 | CB | ASP | A | 332 | 26.640 | 19.752 | 16.090 | 1.00 | 19.49 | A |
| ATOM | 1570 | CG | ASP | A | 332 | 26.835 | 18.254 | 16.228 | 1.00 | 22.57 | A |
| ATOM | 1571 | OD1 | ASP | A | 332 | 26.695 | 17.528 | 15.222 | 1.00 | 23.71 | A |
| ATOM | 1572 | OD2 | ASP | A | 332 | 27.136 | 17.803 | 17.355 | 1.00 | 25.43 | A |
| ATOM | 1573 | C | ASP | A | 332 | 27.311 | 20.053 | 13.689 | 1.00 | 16.67 | A |
| ATOM | 1574 | O | ASP | A | 332 | 28.483 | 20.038 | 14.065 | 1.00 | 15.11 | A |
| ATOM | 1575 | N | GLY | A | 333 | 26.959 | 19.960 | 12.410 | 1.00 | 15.38 | A |
| ATOM | 1576 | CA | GLY | A | 333 | 27.974 | 19.897 | 11.375 | 1.00 | 15.75 | A |
| ATOM | 1577 | C | GLY | A | 333 | 28.344 | 18.547 | 10.796 | 1.00 | 13.57 | A |
| ATOM | 1578 | O | GLY | A | 333 | 27.752 | 17.513 | 11.111 | 1.00 | 14.77 | A |
| ATOM | 1579 | N | VAL | A | 334 | 29.346 | 18.580 | 9.924 | 1.00 | 11.52 | A |
| ATOM | 1580 | CA | VAL | A | 334 | 29.844 | 17.391 | 9.254 | 1.00 | 10.99 | A |
| ATOM | 1581 | CB | VAL | A | 334 | 30.746 | 17.791 | 8.063 | 1.00 | 9.62 | A |
| ATOM | 1582 | CG1 | VAL | A | 334 | 31.534 | 16.585 | 7.549 | 1.00 | 11.92 | A |
| ATOM | 1583 | CG2 | VAL | A | 334 | 29.879 | 18.366 | 6.952 | 1.00 | 12.03 | A |
| ATOM | 1584 | C | VAL | A | 334 | 30.614 | 16.499 | 10.218 | 1.00 | 11.60 | A |
| ATOM | 1585 | O | VAL | A | 334 | 31.450 | 16.965 | 10.989 | 1.00 | 12.63 | A |
| ATOM | 1586 | N | GLY | A | 335 | 30.301 | 15.209 | 10.181 | 1.00 | 12.25 | A |
| ATOM | 1587 | CA | GLY | A | 335 | 30.975 | 14.252 | 11.036 | 1.00 | 12.89 | A |
| ATOM | 1588 | C | GLY | A | 335 | 31.193 | 12.971 | 10.259 | 1.00 | 13.23 | A |
| ATOM | 1589 | O | GLY | A | 335 | 30.982 | 12.931 | 9.048 | 1.00 | 13.01 | A |
| ATOM | 1590 | N | ASP | A | 336 | 31.618 | 11.916 | 10.938 | 1.00 | 15.14 | A |
| ATOM | 1591 | CA | ASP | A | 336 | 31.834 | 10.660 | 10.244 | 1.00 | 16.51 | A |
| ATOM | 1592 | CB | ASP | A | 336 | 32.956 | 9.870 | 10.911 | 1.00 | 17.22 | A |
| ATOM | 1593 | CG | ASP | A | 336 | 34.318 | 10.457 | 10.610 | 1.00 | 19.47 | A |
| ATOM | 1594 | OD1 | ASP | A | 336 | 34.936 | 11.045 | 11.523 | 1.00 | 20.13 | A |
| ATOM | 1595 | OD2 | ASP | A | 336 | 34.753 | 10.345 | 9.443 | 1.00 | 19.26 | A |
| ATOM | 1596 | C | ASP | A | 336 | 30.561 | 9.835 | 10.172 | 1.00 | 16.78 | A |
| ATOM | 1597 | O | ASP | A | 336 | 29.688 | 9.936 | 11.034 | 1.00 | 16.77 | A |
| ATOM | 1598 | N | ALA | A | 337 | 30.451 | 9.039 | 9.116 | 1.00 | 16.17 | A |
| ATOM | 1599 | CA | ALA | A | 337 | 29.285 | 8.195 | 8.920 | 1.00 | 17.98 | A |
| ATOM | 1600 | CB | ALA | A | 337 | 29.267 | 7.651 | 7.497 | 1.00 | 17.82 | A |
| ATOM | 1601 | C | ALA | A | 337 | 29.322 | 7.053 | 9.926 | 1.00 | 19.32 | A |
| ATOM | 1602 | O | ALA | A | 337 | 30.376 | 6.472 | 10.181 | 1.00 | 18.99 | A |
| ATOM | 1603 | N | LYS | A | 338 | 28.163 | 6.738 | 10.490 | 1.00 | 20.19 | A |
| ATOM | 1604 | CA | LYS | A | 338 | 28.053 | 5.676 | 11.479 | 1.00 | 22.21 | A |
| ATOM | 1605 | CB | LYS | A | 338 | 27.738 | 6.279 | 12.850 | 1.00 | 23.47 | A |
| ATOM | 1606 | CG | LYS | A | 338 | 28.784 | 7.255 | 13.360 | 1.00 | 26.58 | A |
| ATOM | 1607 | CD | LYS | A | 338 | 30.111 | 6.561 | 13.623 | 1.00 | 29.32 | A |
| ATOM | 1608 | CE | LYS | A | 338 | 31.150 | 7.544 | 14.142 | 1.00 | 32.11 | A |
| ATOM | 1609 | NZ | LYS | A | 338 | 32.439 | 6.871 | 14.460 | 1.00 | 34.51 | A |
| ATOM | 1610 | C | LYS | A | 338 | 26.946 | 4.702 | 11.099 | 1.00 | 23.93 | A |
| ATOM | 1611 | O | LYS | A | 338 | 25.977 | 5.080 | 10.437 | 1.00 | 22.40 | A |
| ATOM | 1612 | N | ASP | A | 339 | 27.093 | 3.447 | 11.508 | 1.00 | 25.44 | A |
| ATOM | 1613 | CA | ASP | A | 339 | 26.068 | 2.452 | 11.228 | 1.00 | 27.67 | A |
| ATOM | 1614 | CB | ASP | A | 339 | 26.693 | 1.085 | 10.924 | 1.00 | 29.98 | A |
| ATOM | 1615 | CG | ASP | A | 339 | 27.592 | .584 | 12.043 | 1.00 | 32.94 | A |
| ATOM | 1616 | OD1 | ASP | A | 339 | 27.427 | 1.025 | 13.201 | 1.00 | 33.12 | A |
| ATOM | 1617 | OD2 | ASP | A | 339 | 28.462 | -.267 | 11.761 | 1.00 | 36.58 | A |
| ATOM | 1618 | C | ASP | A | 339 | 25.169 | 2.347 | 12.456 | 1.00 | 28.80 | A |
| ATOM | 1619 | O | ASP | A | 339 | 24.424 | 1.352 | 12.570 | 1.00 | 28.88 | A |
| ATOM | 1620 | OXT | ASP | A | 339 | 25.220 | 3.279 | 13.289 | 1.00 | 28.59 | A |
| ATOM | 1621 | CB | PRO | | 1519 | 24.486 | 50.430 | -.203 | .50 | 37.27 | AC1 |
| ATOM | 1622 | CG | PRO | | 1519 | 24.699 | 51.944 | -.398 | .50 | 37.06 | AC1 |
| ATOM | 1623 | C | PRO | | 1519 | 24.307 | 49.154 | 1.952 | .50 | 35.98 | AC1 |
| ATOM | 1624 | O | PRO | | 1519 | 25.171 | 48.407 | 1.497 | .50 | 37.38 | AC1 |
| ATOM | 1625 | N | PRO | | 1519 | 24.293 | 51.611 | 1.883 | .50 | 34.39 | AC1 |
| ATOM | 1626 | CD | PRO | | 1519 | 25.117 | 52.443 | .989 | .50 | 33.96 | AC1 |
| ATOM | 1627 | CA | PRO | | 1519 | 23.845 | 50.392 | 1.173 | .50 | 35.12 | AC1 |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1628 | N | THR | B1520 | 23.744 | 48.961 | 3.142 | 1.00 | 35.07 | B |
| ATOM | 1629 | CA | THR | B1520 | 24.098 | 47.838 | 4.013 | 1.00 | 33.12 | B |
| ATOM | 1630 | CB | THR | B1520 | 23.242 | 47.855 | 5.296 | 1.00 | 33.72 | B |
| ATOM | 1631 | OG1 | THR | B1520 | 21.871 | 47.557 | 4.982 | 1.00 | 33.68 | B |
| ATOM | 1632 | CG2 | THR | B1520 | 23.307 | 49.243 | 5.942 | 1.00 | 34.95 | B |
| ATOM | 1633 | C | THR | B1520 | 23.952 | 46.477 | 3.357 | 1.00 | 31.94 | B |
| ATOM | 1634 | O | THR | B1520 | 24.698 | 45.547 | 3.676 | 1.00 | 31.26 | B |
| ATOM | 1635 | N | LEU | B1521 | 23.026 | 46.379 | 2.411 | 1.00 | 28.07 | B |
| ATOM | 1636 | CA | LEU | B1521 | 22.780 | 45.125 | 1.720 | 1.00 | 27.74 | B |
| ATOM | 1637 | CB | LEU | B1521 | 21.495 | 45.232 | .896 | 1.00 | 27.44 | B |
| ATOM | 1638 | CG | LEU | B1521 | 20.189 | 45.382 | 1.680 | 1.00 | 27.21 | B |
| ATOM | 1639 | CD1 | LEU | B1521 | 19.046 | 45.662 | .717 | 1.00 | 28.85 | B |
| ATOM | 1640 | CD2 | LEU | B1521 | 19.916 | 44.121 | 2.486 | 1.00 | 27.53 | B |
| ATOM | 1641 | C | LEU | B1521 | 23.899 | 44.613 | .817 | 1.00 | 26.48 | B |
| ATOM | 1642 | O | LEU | B1521 | 23.957 | 43.416 | .532 | 1.00 | 26.28 | B |
| ATOM | 1643 | N | LEU | B1522 | 24.783 | 45.500 | .373 | 1.00 | 25.12 | B |
| ATOM | 1644 | CA | LEU | B1522 | 25.854 | 45.093 | -.529 | 1.00 | 24.52 | B |
| ATOM | 1645 | CB | LEU | B1522 | 25.976 | 46.115 | -1.662 | 1.00 | 26.00 | B |
| ATOM | 1646 | CG | LEU | B1522 | 24.681 | 46.354 | -2.447 | 1.00 | 27.30 | B |
| ATOM | 1647 | CD1 | LEU | B1522 | 24.911 | 47.429 | -3.496 | 1.00 | 28.30 | B |
| ATOM | 1648 | CD2 | LEU | B1522 | 24.221 | 45.056 | -3.097 | 1.00 | 26.47 | B |
| ATOM | 1649 | C | LEU | B1522 | 27.221 | 44.871 | .115 | 1.00 | 23.01 | B |
| ATOM | 1650 | O | LEU | B1522 | 28.192 | 44.588 | -.584 | 1.00 | 23.87 | B |
| ATOM | 1651 | N | GLY | B1523 | 27.303 | 44.997 | 1.436 | 1.00 | 21.25 | B |
| ATOM | 1652 | CA | GLY | B1523 | 28.572 | 44.787 | 2.114 | 1.00 | 19.07 | B |
| ATOM | 1653 | C | GLY | B1523 | 28.527 | 43.565 | 3.013 | 1.00 | 16.93 | B |
| ATOM | 1654 | O | GLY | B1523 | 27.592 | 42.769 | 2.933 | 1.00 | 18.20 | B |
| ATOM | 1655 | N | PHE | B1524 | 29.531 | 43.414 | 3.872 | 1.00 | 15.85 | B |
| ATOM | 1656 | CA | PHE | B1524 | 29.590 | 42.278 | 4.791 | 1.00 | 13.68 | B |
| ATOM | 1657 | CB | PHE | B1524 | 31.027 | 41.762 | 4.942 | 1.00 | 13.38 | B |
| ATOM | 1658 | CG | PHE | B1524 | 31.521 | 40.956 | 3.776 | 1.00 | 12.94 | B |
| ATOM | 1659 | CD1 | PHE | B1524 | 32.085 | 41.577 | 2.667 | 1.00 | 14.58 | B |
| ATOM | 1660 | CD2 | PHE | B1524 | 31.440 | 39.568 | 3.799 | 1.00 | 13.15 | B |
| ATOM | 1661 | CE1 | PHE | B1524 | 32.567 | 40.825 | 1.594 | 1.00 | 12.21 | B |
| ATOM | 1662 | CE2 | PHE | B1524 | 31.914 | 38.805 | 2.734 | 1.00 | 13.77 | B |
| ATOM | 1663 | CZ | PHE | B1524 | 32.482 | 39.437 | 1.628 | 1.00 | 14.06 | B |
| ATOM | 1664 | C | PHE | B1524 | 29.088 | 42.622 | 6.188 | 1.00 | 12.65 | B |
| ATOM | 1665 | O | PHE | B1524 | 29.194 | 43.762 | 6.635 | 1.00 | 13.98 | B |
| ATOM | 1666 | N | HIS | B1525 | 28.547 | 41.613 | 6.865 | 1.00 | 11.84 | B |
| ATOM | 1667 | CA | HIS | B1525 | 28.078 | 41.733 | 8.241 | 1.00 | 13.15 | B |
| ATOM | 1668 | CB | HIS | B1525 | 26.553 | 41.694 | 8.327 | 1.00 | 15.13 | B |
| ATOM | 1669 | CG | HIS | B1525 | 25.881 | 42.936 | 7.844 | 1.00 | 18.82 | B |
| ATOM | 1670 | CD2 | HIS | B1525 | 25.345 | 43.978 | 8.521 | 1.00 | 20.71 | B |
| ATOM | 1671 | ND1 | HIS | B1525 | 25.675 | 43.198 | 6.507 | 1.00 | 23.42 | B |
| ATOM | 1672 | CE1 | HIS | B1525 | 25.036 | 44.349 | 6.382 | 1.00 | 21.27 | B |
| ATOM | 1673 | NE2 | HIS | B1525 | 24.824 | 44.842 | 7.589 | 1.00 | 22.01 | B |
| ATOM | 1674 | C | HIS | B1525 | 28.608 | 40.506 | 8.977 | 1.00 | 12.75 | B |
| ATOM | 1675 | O | HIS | B1525 | 28.847 | 39.468 | 8.358 | 1.00 | 12.86 | B |
| ATOM | 1676 | N | THR | B1526 | 28.812 | 40.612 | 10.283 | 1.00 | 11.64 | B |
| ATOM | 1677 | CA | THR | B1526 | 29.261 | 39.439 | 11.023 | 1.00 | 11.86 | B |
| ATOM | 1678 | CB | THR | B1526 | 29.661 | 39.773 | 12.471 | 1.00 | 12.84 | B |
| ATOM | 1679 | OG1 | THR | B1526 | 28.529 | 40.315 | 13.165 | 1.00 | 14.05 | B |
| ATOM | 1680 | CG2 | THR | B1526 | 30.808 | 40.768 | 12.495 | 1.00 | 12.72 | B |
| ATOM | 1681 | C | THR | B1526 | 28.037 | 38.533 | 11.065 | 1.00 | 12.89 | B |
| ATOM | 1682 | O | THR | B1526 | 26.927 | 38.979 | 10.777 | 1.00 | 13.46 | B |
| ATOM | 1683 | N | ALA | B1527 | 28.222 | 37.267 | 11.419 | 1.00 | 11.46 | B |
| ATOM | 1684 | CA | ALA | B1527 | 27.090 | 36.355 | 11.486 | 1.00 | 14.41 | B |
| ATOM | 1685 | CB | ALA | B1527 | 27.577 | 34.923 | 11.695 | 1.00 | 12.82 | B |
| ATOM | 1686 | C | ALA | B1527 | 26.144 | 36.771 | 12.614 | 1.00 | 15.41 | B |
| ATOM | 1687 | O | ALA | B1527 | 25.014 | 36.286 | 12.695 | 1.00 | 17.98 | B |
| ATOM | 1688 | N | SER | B1528 | 26.615 | 37.667 | 13.480 | 1.00 | 16.56 | B |
| ATOM | 1689 | CA | SER | B1528 | 25.813 | 38.174 | 14.593 | 1.00 | 19.61 | B |
| ATOM | 1690 | CB | SER | B1528 | 26.701 | 38.453 | 15.816 | 1.00 | 19.90 | B |
| ATOM | 1691 | OG | SER | B1528 | 27.833 | 39.242 | 15.479 | 1.00 | 23.75 | B |
| ATOM | 1692 | C | SER | B1528 | 25.045 | 39.438 | 14.197 | 1.00 | 20.84 | B |
| ATOM | 1693 | O | SER | B1528 | 24.355 | 40.041 | 15.025 | 1.00 | 22.21 | B |
| ATOM | 1694 | N | GLY | B1529 | 25.177 | 39.840 | 12.934 | 1.00 | 20.05 | B |
| ATOM | 1695 | CA | GLY | B1529 | 24.463 | 41.009 | 12.440 | 1.00 | 20.14 | B |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1696 | C | GLY | B1529 | 25.170 | 42.352 | 12.501 | 1.00 | 19.33 | B |
| ATOM | 1697 | O | GLY | B1529 | 24.563 | 43.386 | 12.206 | 1.00 | 20.61 | B |
| ATOM | 1698 | N | LYS | B1530 | 26.444 | 42.355 | 12.873 | 1.00 | 17.30 | B |
| ATOM | 1699 | CA | LYS | B1530 | 27.201 | 43.601 | 12.970 | 1.00 | 17.58 | B |
| ATOM | 1700 | CB | LYS | B1530 | 28.286 | 43.475 | 14.038 | 1.00 | 17.52 | B |
| ATOM | 1701 | CG | LYS | B1530 | 27.772 | 43.081 | 15.411 | 1.00 | 21.01 | B |
| ATOM | 1702 | CD | LYS | B1530 | 28.925 | 42.887 | 16.381 | 1.00 | 23.76 | B |
| ATOM | 1703 | CE | LYS | B1530 | 28.419 | 42.487 | 17.756 | 1.00 | 26.60 | B |
| ATOM | 1704 | NZ | LYS | B1530 | 27.538 | 41.296 | 17.669 | 1.00 | 30.15 | B |
| ATOM | 1705 | C | LYS | B1530 | 27.853 | 43.992 | 11.647 | 1.00 | 18.75 | B |
| ATOM | 1706 | O | LYS | B1530 | 28.533 | 43.182 | 11.018 | 1.00 | 17.86 | B |
| ATOM | 1707 | N | LYS | B1531 | 27.649 | 45.237 | 11.228 | 1.00 | 17.05 | B |
| ATOM | 1708 | CA | LYS | B1531 | 28.251 | 45.718 | 9.991 | 1.00 | 19.95 | B |
| ATOM | 1709 | CB | LYS | B1531 | 27.836 | 47.172 | 9.727 | 1.00 | 22.55 | B |
| ATOM | 1710 | CG | LYS | B1531 | 28.565 | 47.851 | 8.567 | 1.00 | 28.55 | B |
| ATOM | 1711 | CD | LYS | B1531 | 28.007 | 47.435 | 7.215 | 1.00 | 34.63 | B |
| ATOM | 1712 | CE | LYS | B1531 | 28.704 | 48.189 | 6.086 | 1.00 | 36.55 | B |
| ATOM | 1713 | NZ | LYS | B1531 | 28.094 | 47.921 | 4.752 | 1.00 | 39.45 | B |
| ATOM | 1714 | C | LYS | B1531 | 29.767 | 45.629 | 10.134 | 1.00 | 19.45 | B |
| ATOM | 1715 | O | LYS | B1531 | 30.314 | 45.892 | 11.206 | 1.00 | 20.19 | B |
| ATOM | 1716 | N | VAL | B1532 | 30.446 | 45.235 | 9.062 | 1.00 | 19.36 | B |
| ATOM | 1717 | CA | VAL | B1532 | 31.899 | 45.140 | 9.091 | 1.00 | 19.78 | B |
| ATOM | 1718 | CB | VAL | B1532 | 32.411 | 43.938 | 8.268 | 1.00 | 19.96 | B |
| ATOM | 1719 | CG1 | VAL | B1532 | 33.930 | 43.987 | 8.162 | 1.00 | 19.38 | B |
| ATOM | 1720 | CG2 | VAL | B1532 | 31.970 | 42.638 | 8.919 | 1.00 | 19.54 | B |
| ATOM | 1721 | C | VAL | B1532 | 32.469 | 46.419 | 8.496 | 1.00 | 20.72 | B |
| ATOM | 1722 | O | VAL | B1532 | 32.213 | 46.738 | 7.337 | 1.00 | 22.21 | B |
| ATOM | 1723 | N | LYS | B1533 | 33.234 | 47.156 | 9.295 | 1.00 | 22.24 | B |
| ATOM | 1724 | CA | LYS | B1533 | 33.826 | 48.405 | 8.829 | 1.00 | 25.01 | B |
| ATOM | 1725 | CB | LYS | B1533 | 34.009 | 49.375 | 10.000 | 1.00 | 29.14 | B |
| ATOM | 1726 | CG | LYS | B1533 | 32.705 | 49.823 | 10.635 | 1.00 | 33.73 | B |
| ATOM | 1727 | CD | LYS | B1533 | 32.941 | 50.800 | 11.776 | 1.00 | 38.58 | B |
| ATOM | 1728 | CE | LYS | B1533 | 33.556 | 52.098 | 11.279 | 1.00 | 40.70 | B |
| ATOM | 1729 | NZ | LYS | B1533 | 33.790 | 53.054 | 12.396 | 1.00 | 43.43 | B |
| ATOM | 1730 | C | LYS | B1533 | 35.166 | 48.173 | 8.140 | 1.00 | 24.17 | B |
| ATOM | 1731 | O | LYS | B1533 | 35.982 | 47.369 | 8.592 | 1.00 | 24.48 | B |
| ATOM | 1732 | N | ILE | B1534 | 35.374 | 48.882 | 7.037 | 1.00 | 23.24 | B |
| ATOM | 1733 | CA | ILE | B1534 | 36.605 | 48.775 | 6.264 | 1.00 | 24.18 | B |
| ATOM | 1734 | CB | ILE | B1534 | 36.326 | 48.206 | 4.856 | 1.00 | 25.08 | B |
| ATOM | 1735 | CG2 | ILE | B1534 | 37.633 | 48.049 | 4.090 | 1.00 | 25.82 | B |
| ATOM | 1736 | CG1 | ILE | B1534 | 35.604 | 46.860 | 4.967 | 1.00 | 25.24 | B |
| ATOM | 1737 | CD1 | ILE | B1534 | 35.219 | 46.258 | 3.627 | 1.00 | 25.28 | B |
| ATOM | 1738 | C | ILE | B1534 | 37.204 | 50.169 | 6.111 | 1.00 | 23.73 | B |
| ATOM | 1739 | O | ILE | B1534 | 36.559 | 51.064 | 5.569 | 1.00 | 23.27 | B |
| ATOM | 1740 | N | ALA | B1535 | 38.430 | 50.351 | 6.591 | 1.00 | 24.35 | B |
| ATOM | 1741 | CA | ALA | B1535 | 39.100 | 51.645 | 6.489 | 1.00 | 24.68 | B |
| ATOM | 1742 | CB | ALA | B1535 | 40.416 | 51.615 | 7.254 | 1.00 | 24.73 | B |
| ATOM | 1743 | C | ALA | B1535 | 39.356 | 51.984 | 5.025 | 1.00 | 26.08 | B |
| ATOM | 1744 | O | ALA | B1535 | 39.755 | 51.121 | 4.244 | 1.00 | 25.25 | B |
| ATOM | 1745 | N | LYS | B1536 | 39.125 | 53.242 | 4.655 | 1.00 | 26.80 | B |
| ATOM | 1746 | CA | LYS | B1536 | 39.335 | 53.681 | 3.279 | 1.00 | 27.59 | B |
| ATOM | 1747 | CB | LYS | B1536 | 39.040 | 55.178 | 3.145 | 1.00 | 30.55 | B |
| ATOM | 1748 | CG | LYS | B1536 | 39.898 | 56.068 | 4.032 | 1.00 | 34.62 | B |
| ATOM | 1749 | CD | LYS | B1536 | 39.565 | 57.545 | 3.836 | 1.00 | 38.95 | B |
| ATOM | 1750 | CE | LYS | B1536 | 39.832 | 57.994 | 2.403 | 1.00 | 41.45 | B |
| ATOM | 1751 | NZ | LYS | B1536 | 39.531 | 59.441 | 2.196 | 1.00 | 43.50 | B |
| ATOM | 1752 | C | LYS | B1536 | 40.762 | 53.393 | 2.819 | 1.00 | 25.80 | B |
| ATOM | 1753 | O | LYS | B1536 | 40.993 | 53.094 | 1.646 | 1.00 | 26.01 | B |
| ATOM | 1754 | N | GLU | B1537 | 41.716 | 53.485 | 3.741 | 1.00 | 24.83 | B |
| ATOM | 1755 | CA | GLU | B1537 | 43.110 | 53.219 | 3.409 | 1.00 | 24.45 | B |
| ATOM | 1756 | CB | GLU | B1537 | 44.029 | 53.519 | 4.600 | 1.00 | 27.10 | B |
| ATOM | 1757 | CG | GLU | B1537 | 44.110 | 54.984 | 5.023 | 1.00 | 31.85 | B |
| ATOM | 1758 | CD | GLU | B1537 | 42.846 | 55.479 | 5.698 | 1.00 | 35.28 | B |
| ATOM | 1759 | OE1 | GLU | B1537 | 42.257 | 54.715 | 6.492 | 1.00 | 35.95 | B |
| ATOM | 1760 | OE2 | GLU | B1537 | 42.451 | 56.639 | 5.449 | 1.00 | 37.98 | B |
| ATOM | 1761 | C | GLU | B1537 | 43.281 | 51.756 | 3.007 | 1.00 | 22.80 | B |
| ATOM | 1762 | O | GLU | B1537 | 44.055 | 51.440 | 2.106 | 1.00 | 22.40 | B |
| ATOM | 1763 | N | SER | B1538 | 42.556 | 50.866 | 3.680 | 1.00 | 21.37 | B |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1764 | CA | SER | B1538 | 42.641 | 49.440 | 3.382 | 1.00 | 20.86 | B |
| ATOM | 1765 | CB | SER | B1538 | 41.781 | 48.644 | 4.366 | 1.00 | 21.09 | B |
| ATOM | 1766 | OG | SER | B1538 | 42.283 | 48.776 | 5.684 | 1.00 | 23.23 | B |
| ATOM | 1767 | C | SER | B1538 | 42.211 | 49.134 | 1.949 | 1.00 | 20.08 | B |
| ATOM | 1768 | O | SER | B1538 | 42.845 | 48.333 | 1.259 | 1.00 | 18.25 | B |
| ATOM | 1769 | N | LEU | B1539 | 41.130 | 49.769 | 1.508 | 1.00 | 19.51 | B |
| ATOM | 1770 | CA | LEU | B1539 | 40.635 | 49.577 | .153 | 1.00 | 20.82 | B |
| ATOM | 1771 | CB | LEU | B1539 | 39.276 | 50.260 | -.013 | 1.00 | 22.90 | B |
| ATOM | 1772 | CG | LEU | B1539 | 38.104 | 49.588 | .708 | 1.00 | 24.42 | B |
| ATOM | 1773 | CD1 | LEU | B1539 | 36.933 | 50.553 | .816 | 1.00 | 26.46 | B |
| ATOM | 1774 | CD2 | LEU | B1539 | 37.705 | 48.326 | -.043 | 1.00 | 25.08 | B |
| ATOM | 1775 | C | LEU | B1539 | 41.638 | 50.159 | -.839 | 1.00 | 20.41 | B |
| ATOM | 1776 | O | LEU | B1539 | 41.880 | 49.588 | -1.903 | 1.00 | 20.85 | B |
| ATOM | 1777 | N | ASP | B1540 | 42.230 | 51.293 | -.481 | 1.00 | 20.18 | B |
| ATOM | 1778 | CA | ASP | B1540 | 43.207 | 51.936 | -1.348 | 1.00 | 20.28 | B |
| ATOM | 1779 | CB | ASP | B1540 | 43.594 | 53.305 | -.776 | 1.00 | 23.88 | B |
| ATOM | 1780 | CG | ASP | B1540 | 44.384 | 54.147 | -1.761 | 1.00 | 26.54 | B |
| ATOM | 1781 | OD1 | ASP | B1540 | 43.862 | 54.414 | -2.865 | 1.00 | 29.37 | B |
| ATOM | 1782 | OD2 | ASP | B1540 | 45.522 | 54.547 | -1.435 | 1.00 | 30.42 | B |
| ATOM | 1783 | C | ASP | B1540 | 44.453 | 51.060 | -1.490 | 1.00 | 20.02 | B |
| ATOM | 1784 | O | ASP | B1540 | 45.038 | 50.967 | -2.569 | 1.00 | 20.33 | B |
| ATOM | 1785 | N | LYS | B1541 | 44.851 | 50.413 | -.399 | 1.00 | 19.20 | B |
| ATOM | 1786 | CA | LYS | B1541 | 46.035 | 49.556 | -.405 | 1.00 | 19.77 | B |
| ATOM | 1787 | CB | LYS | B1541 | 46.356 | 49.089 | 1.019 | 1.00 | 21.48 | B |
| ATOM | 1788 | CG | LYS | B1541 | 46.809 | 50.212 | 1.946 | 1.00 | 24.88 | B |
| ATOM | 1789 | CD | LYS | B1541 | 46.941 | 49.733 | 3.383 | 1.00 | 26.41 | B |
| ATOM | 1790 | CE | LYS | B1541 | 47.320 | 50.878 | 4.309 | 1.00 | 28.15 | B |
| ATOM | 1791 | NZ | LYS | B1541 | 47.277 | 50.469 | 5.743 | 1.00 | 31.20 | B |
| ATOM | 1792 | C | LYS | B1541 | 45.918 | 48.342 | -1.328 | 1.00 | 19.38 | B |
| ATOM | 1793 | O | LYS | B1541 | 46.923 | 47.879 | -1.873 | 1.00 | 19.13 | B |
| ATOM | 1794 | N | VAL | B1542 | 44.701 | 47.836 | -1.514 | 1.00 | 18.52 | B |
| ATOM | 1795 | CA | VAL | B1542 | 44.485 | 46.669 | -2.369 | 1.00 | 18.69 | B |
| ATOM | 1796 | CB | VAL | B1542 | 43.539 | 45.650 | -1.685 | 1.00 | 18.33 | B |
| ATOM | 1797 | CG1 | VAL | B1542 | 44.121 | 45.214 | -.359 | 1.00 | 20.04 | B |
| ATOM | 1798 | CG2 | VAL | B1542 | 42.162 | 46.264 | -1.483 | 1.00 | 19.59 | B |
| ATOM | 1799 | C | VAL | B1542 | 43.906 | 47.015 | -3.740 | 1.00 | 18.77 | B |
| ATOM | 1800 | O | VAL | B1542 | 43.557 | 46.123 | -4.513 | 1.00 | 19.16 | B |
| ATOM | 1801 | N | LYS | B1543 | 43.822 | 48.309 | -4.042 | 1.00 | 20.01 | B |
| ATOM | 1802 | CA | LYS | B1543 | 43.268 | 48.784 | -5.312 | 1.00 | 21.69 | B |
| ATOM | 1803 | CB | LYS | B1543 | 43.488 | 50.299 | -5.444 | 1.00 | 23.55 | B |
| ATOM | 1804 | CG | LYS | B1543 | 44.954 | 50.700 | -5.482 | 1.00 | 28.56 | B |
| ATOM | 1805 | CD | LYS | B1543 | 45.158 | 52.205 | -5.344 | 1.00 | 32.47 | B |
| ATOM | 1806 | CE | LYS | B1543 | 44.767 | 52.961 | -6.600 | 1.00 | 35.65 | B |
| ATOM | 1807 | NZ | LYS | B1543 | 45.188 | 54.390 | -6.512 | 1.00 | 38.75 | B |
| ATOM | 1808 | C | LYS | B1543 | 43.808 | 48.090 | -6.564 | 1.00 | 20.66 | B |
| ATOM | 1809 | O | LYS | B1543 | 43.067 | 47.879 | -7.525 | 1.00 | 21.57 | B |
| ATOM | 1810 | N | ASN | B1544 | 45.088 | 47.732 | -6.556 | 1.00 | 20.57 | B |
| ATOM | 1811 | CA | ASN | B1544 | 45.698 | 47.090 | -7.720 | 1.00 | 19.97 | B |
| ATOM | 1812 | CB | ASN | B1544 | 47.010 | 47.795 | -8.077 | 1.00 | 22.42 | B |
| ATOM | 1813 | CG | ASN | B1544 | 46.817 | 49.263 | -8.392 | 1.00 | 24.61 | B |
| ATOM | 1814 | OD1 | ASN | B1544 | 46.018 | 49.624 | -9.257 | 1.00 | 26.96 | B |
| ATOM | 1815 | ND2 | ASN | B1544 | 47.553 | 50.121 | -7.692 | 1.00 | 26.00 | B |
| ATOM | 1816 | C | ASN | B1544 | 45.974 | 45.598 | -7.566 | 1.00 | 18.50 | B |
| ATOM | 1817 | O | ASN | B1544 | 46.583 | 44.989 | -8.440 | 1.00 | 17.10 | B |
| ATOM | 1818 | N | LEU | B1545 | 45.518 | 45.007 | -6.469 | 1.00 | 17.20 | B |
| ATOM | 1819 | CA | LEU | B1545 | 45.762 | 43.591 | -6.217 | 1.00 | 16.66 | B |
| ATOM | 1820 | CB | LEU | B1545 | 45.054 | 43.156 | -4.929 | 1.00 | 16.31 | B |
| ATOM | 1821 | CG | LEU | B1545 | 45.166 | 41.665 | -4.598 | 1.00 | 16.59 | B |
| ATOM | 1822 | CD1 | LEU | B1545 | 46.622 | 41.300 | -4.352 | 1.00 | 16.66 | B |
| ATOM | 1823 | CD2 | LEU | B1545 | 44.319 | 41.347 | -3.379 | 1.00 | 17.51 | B |
| ATOM | 1824 | C | LEU | B1545 | 45.362 | 42.637 | -7.336 | 1.00 | 16.69 | B |
| ATOM | 1825 | O | LEU | B1545 | 46.047 | 41.641 | -7.579 | 1.00 | 16.64 | B |
| ATOM | 1826 | N | PHE | B1546 | 44.258 | 42.932 | -8.014 | 1.00 | 16.22 | B |
| ATOM | 1827 | CA | PHE | B1546 | 43.775 | 42.047 | -9.063 | 1.00 | 17.49 | B |
| ATOM | 1828 | CB | PHE | B1546 | 42.247 | 41.967 | -8.998 | 1.00 | 15.66 | B |
| ATOM | 1829 | CG | PHE | B1546 | 41.737 | 41.417 | -7.699 | 1.00 | 11.70 | B |
| ATOM | 1830 | CD1 | PHE | B1546 | 41.945 | 40.081 | -7.366 | 1.00 | 13.72 | B |
| ATOM | 1831 | CD2 | PHE | B1546 | 41.099 | 42.243 | -6.780 | 1.00 | 13.72 | B |

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ATOM   1832  CE1 PHE B1546      41.530  39.577  -6.137  1.00 14.70      B
ATOM   1833  CE2 PHE B1546      40.680  41.748  -5.544  1.00 14.99      B
ATOM   1834  CZ  PHE B1546      40.897  40.413  -5.223  1.00 14.37      B
ATOM   1835  C   PHE B1546      44.225  42.384 -10.474  1.00 18.64      B
ATOM   1836  O   PHE B1546      43.774  41.763 -11.432  1.00 19.17      B
ATOM   1837  N   ASP B1547      45.116  43.358 -10.609  1.00 19.30      B
ATOM   1838  CA  ASP B1547      45.602  43.709 -11.934  1.00 22.97      B
ATOM   1839  CB  ASP B1547      46.481  44.962 -11.901  1.00 25.04      B
ATOM   1840  CG  ASP B1547      45.736  46.193 -11.447  1.00 28.33      B
ATOM   1841  OD1 ASP B1547      44.491  46.212 -11.535  1.00 30.07      B
ATOM   1842  OD2 ASP B1547      46.408  47.155 -11.016  1.00 32.49      B
ATOM   1843  C   ASP B1547      46.437  42.557 -12.464  1.00 22.48      B
ATOM   1844  O   ASP B1547      47.139  41.882 -11.712  1.00 24.30      B
ATOM   1845  N   GLU B1548      46.346  42.329 -13.765  1.00 22.96      B
ATOM   1846  CA  GLU B1548      47.118  41.288 -14.413  1.00 22.18      B
ATOM   1847  CB  GLU B1548      46.195  40.276 -15.095  1.00 22.32      B
ATOM   1848  CG  GLU B1548      45.388  39.459 -14.099  1.00 21.84      B
ATOM   1849  CD  GLU B1548      44.480  38.444 -14.759  1.00 21.72      B
ATOM   1850  OE1 GLU B1548      43.684  38.844 -15.632  1.00 20.97      B
ATOM   1851  OE2 GLU B1548      44.558  37.251 -14.396  1.00 23.36      B
ATOM   1852  C   GLU B1548      47.981  42.024 -15.422  1.00 23.17      B
ATOM   1853  O   GLU B1548      47.867  41.829 -16.633  1.00 24.15      B
ATOM   1854  N   LYS B1549      48.825  42.901 -14.886  1.00 22.17      B
ATOM   1855  CA  LYS B1549      49.742  43.713 -15.671  1.00 22.56      B
ATOM   1856  CB  LYS B1549      50.412  44.764 -14.781  1.00 24.49      B
ATOM   1857  CG  LYS B1549      49.486  45.834 -14.236  1.00 29.70      B
ATOM   1858  CD  LYS B1549      49.077  46.801 -15.325  1.00 33.15      B
ATOM   1859  CE  LYS B1549      48.328  47.985 -14.745  1.00 36.67      B
ATOM   1860  NZ  LYS B1549      49.149  48.714 -13.739  1.00 40.31      B
ATOM   1861  C   LYS B1549      50.822  42.838 -16.275  1.00 20.74      B
ATOM   1862  O   LYS B1549      51.222  41.832 -15.687  1.00 20.95      B
ATOM   1863  N   GLU B1550      51.295  43.223 -17.452  1.00 19.67      B
ATOM   1864  CA  GLU B1550      52.353  42.472 -18.099  1.00 20.42      B
ATOM   1865  CB  GLU B1550      52.577  42.987 -19.518  1.00 21.71      B
ATOM   1866  CG  GLU B1550      51.559  42.447 -20.510  1.00 25.16      B
ATOM   1867  CD  GLU B1550      51.666  43.101 -21.867  1.00 27.14      B
ATOM   1868  OE1 GLU B1550      52.801  43.271 -22.360  1.00 28.85      B
ATOM   1869  OE2 GLU B1550      50.611  43.440 -22.443  1.00 30.89      B
ATOM   1870  C   GLU B1550      53.610  42.632 -17.258  1.00 20.42      B
ATOM   1871  O   GLU B1550      53.912  43.722 -16.769  1.00 21.55      B
ATOM   1872  N   GLN B1551      54.329  41.532 -17.082  1.00 19.31      B
ATOM   1873  CA  GLN B1551      55.542  41.516 -16.286  1.00 20.35      B
ATOM   1874  CB  GLN B1551      55.559  40.255 -15.422  1.00 19.40      B
ATOM   1875  CG  GLN B1551      54.349  40.114 -14.521  1.00 19.34      B
ATOM   1876  CD  GLN B1551      54.267  41.231 -13.504  1.00 22.39      B
ATOM   1877  OE1 GLN B1551      55.221  41.481 -12.770  1.00 21.26      B
ATOM   1878  NE2 GLN B1551      53.127  41.908 -13.455  1.00 22.77      B
ATOM   1879  C   GLN B1551      56.782  41.541 -17.170  1.00 21.10      B
ATOM   1880  O   GLN B1551      56.683  41.486 -18.395  1.00 21.97      B
ATOM   1881  N   THR B1552      57.949  41.639 -16.544  1.00 22.64      B
ATOM   1882  CA  THR B1552      59.201  41.634 -17.288  1.00 25.11      B
ATOM   1883  CB  THR B1552      60.332  42.316 -16.497  1.00 27.42      B
ATOM   1884  OG1 THR B1552      59.999  43.692 -16.281  1.00 29.24      B
ATOM   1885  CG2 THR B1552      61.645  42.228 -17.265  1.00 27.94      B
ATOM   1886  C   THR B1552      59.567  40.172 -17.505  1.00 25.06      B
ATOM   1887  O   THR B1552      59.769  39.432 -16.545  1.00 25.65      B
ATOM   1888  N   GLY B1553      59.637  39.756 -18.764  1.00 25.65      B
ATOM   1889  CA  GLY B1553      59.967  38.373 -19.057  1.00 25.06      B
ATOM   1890  C   GLY B1553      61.378  38.190 -19.573  1.00 26.56      B
ATOM   1891  O   GLY B1553      61.927  39.065 -20.242  1.00 26.49      B
ATOM   1892  N   SER B1554      61.972  37.046 -19.255  1.00 28.84      B
ATOM   1893  CA  SER B1554      63.325  36.743 -19.702  1.00 30.62      B
ATOM   1894  CB  SER B1554      64.346  37.283 -18.696  1.00 32.10      B
ATOM   1895  OG  SER B1554      64.127  36.745 -17.401  1.00 33.78      B
ATOM   1896  C   SER B1554      63.510  35.238 -19.872  1.00 30.37      B
ATOM   1897  O   SER B1554      62.646  34.475 -19.388  1.00 31.99      B
ATOM   1898  OXT SER B1554      64.523  34.841 -20.486  1.00 33.32      B
ATOM   1899  C   GLY C   1      23.040  64.501  10.728  1.00 25.62      C
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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1900 | O | GLY | C | 1 | 22.550 | 63.402 | 10.981 | 1.00 | 24.58 | C |
| ATOM | 1901 | N | GLY | C | 1 | 23.653 | 64.653 | 13.149 | 1.00 | 26.62 | C |
| ATOM | 1902 | CA | GLY | C | 1 | 23.720 | 65.313 | 11.814 | 1.00 | 25.97 | C |
| ATOM | 1903 | N | SER | C | 2 | 23.029 | 65.034 | 9.509 | 1.00 | 24.78 | C |
| ATOM | 1904 | CA | SER | C | 2 | 22.384 | 64.364 | 8.385 | 1.00 | 25.77 | C |
| ATOM | 1905 | CB | SER | C | 2 | 21.632 | 65.390 | 7.535 | 1.00 | 24.41 | C |
| ATOM | 1906 | OG | SER | C | 2 | 20.677 | 66.091 | 8.309 | 1.00 | 23.97 | C |
| ATOM | 1907 | C | SER | C | 2 | 23.325 | 63.569 | 7.486 | 1.00 | 26.68 | C |
| ATOM | 1908 | O | SER | C | 2 | 22.896 | 63.028 | 6.467 | 1.00 | 25.80 | C |
| ATOM | 1909 | N | MSE | C | 3 | 24.601 | 63.496 | 7.847 | 1.00 | 28.16 | C |
| ATOM | 1910 | CA | MSE | C | 3 | 25.553 | 62.751 | 7.031 | 1.00 | 31.64 | C |
| ATOM | 1911 | CB | MSE | C | 3 | 26.938 | 62.778 | 7.670 | 1.00 | 33.78 | C |
| ATOM | 1912 | CG | MSE | C | 3 | 28.000 | 62.090 | 6.840 | 1.00 | 38.54 | C |
| ATOM | 1913 | SE | MSE | C | 3 | 29.693 | 62.045 | 7.747 | 1.00 | 49.47 | C |
| ATOM | 1914 | CE | MSE | C | 3 | 30.391 | 63.745 | 7.182 | 1.00 | 43.04 | C |
| ATOM | 1915 | C | MSE | C | 3 | 25.087 | 61.305 | 6.881 | 1.00 | 32.89 | C |
| ATOM | 1916 | O | MSE | C | 3 | 24.652 | 60.685 | 7.851 | 1.00 | 32.94 | C |
| ATOM | 1917 | N | GLY | C | 4 | 25.182 | 60.771 | 5.665 | 1.00 | 34.65 | C |
| ATOM | 1918 | CA | GLY | C | 4 | 24.754 | 59.401 | 5.437 | 1.00 | 36.89 | C |
| ATOM | 1919 | C | GLY | C | 4 | 25.681 | 58.384 | 6.070 | 1.00 | 38.07 | C |
| ATOM | 1920 | O | GLY | C | 4 | 26.885 | 58.684 | 6.213 | 1.00 | 38.86 | C |
| ATOM | 1921 | OXT | GLY | C | 4 | 25.207 | 57.277 | 6.411 | 1.00 | 40.87 | C |
| ATOM | 1922 | O | HOH | | 1 | 27.203 | 32.665 | -8.545 | 1.00 | 12.07 | |
| ATOM | 1923 | O | HOH | | 2 | 31.152 | 37.373 | -10.128 | 1.00 | 14.68 | |
| ATOM | 1924 | O | HOH | | 3 | 24.813 | 29.097 | 1.505 | 1.00 | 19.02 | |
| ATOM | 1925 | O | HOH | | 4 | 41.055 | 25.105 | -.319 | 1.00 | 11.16 | |
| ATOM | 1926 | O | HOH | | 5 | 43.681 | 37.645 | 6.233 | 1.00 | 14.81 | |
| ATOM | 1927 | O | HOH | | 6 | 45.327 | 22.607 | 11.105 | 1.00 | 13.75 | |
| ATOM | 1928 | O | HOH | | 7 | 39.600 | 31.034 | -14.585 | 1.00 | 13.20 | |
| ATOM | 1929 | O | HOH | | 8 | 43.640 | 26.446 | -6.581 | 1.00 | 14.05 | |
| ATOM | 1930 | O | HOH | | 9 | 25.339 | 14.708 | -6.366 | 1.00 | 21.76 | |
| ATOM | 1931 | O | HOH | | 10 | 47.852 | 25.013 | 18.123 | 1.00 | 15.00 | |
| ATOM | 1932 | O | HOH | | 11 | 41.038 | 31.746 | -16.720 | 1.00 | 15.00 | |
| ATOM | 1933 | O | HOH | | 12 | 34.703 | 38.853 | -12.674 | 1.00 | 14.66 | |
| ATOM | 1934 | O | HOH | | 13 | 41.935 | 21.373 | -.230 | 1.00 | 15.53 | |
| ATOM | 1935 | O | HOH | | 14 | 33.052 | 8.732 | 7.686 | 1.00 | 17.18 | |
| ATOM | 1936 | O | HOH | | 15 | 29.065 | 32.805 | 23.625 | 1.00 | 22.84 | |
| ATOM | 1937 | O | HOH | | 16 | 39.100 | 42.813 | 8.664 | 1.00 | 24.97 | |
| ATOM | 1938 | O | HOH | | 17 | 45.225 | 34.430 | -10.500 | 1.00 | 14.90 | |
| ATOM | 1939 | O | HOH | | 18 | 34.758 | 6.368 | 4.080 | 1.00 | 20.01 | |
| ATOM | 1940 | O | HOH | | 19 | 27.240 | 27.751 | 20.443 | 1.00 | 18.69 | |
| ATOM | 1941 | O | HOH | | 20 | 50.907 | 39.282 | -16.750 | 1.00 | 20.51 | |
| ATOM | 1942 | O | HOH | | 21 | 47.270 | 47.282 | -4.465 | 1.00 | 21.63 | |
| ATOM | 1943 | O | HOH | | 22 | 40.136 | 25.218 | 21.558 | 1.00 | 19.04 | |
| ATOM | 1944 | O | HOH | | 23 | 26.144 | 8.662 | 10.277 | 1.00 | 18.32 | |
| ATOM | 1945 | O | HOH | | 24 | 42.725 | 45.381 | -8.655 | 1.00 | 27.15 | |
| ATOM | 1946 | O | HOH | | 25 | 40.507 | 26.175 | -10.534 | 1.00 | 24.50 | |
| ATOM | 1947 | O | HOH | | 26 | 28.530 | 16.165 | 13.719 | 1.00 | 33.54 | |
| ATOM | 1948 | O | HOH | | 27 | 49.779 | 14.277 | 1.640 | 1.00 | 26.13 | |
| ATOM | 1949 | O | HOH | | 28 | 37.754 | 17.604 | 13.513 | 1.00 | 21.28 | |
| ATOM | 1950 | O | HOH | | 29 | 25.719 | 40.907 | 4.909 | 1.00 | 26.13 | |
| ATOM | 1951 | O | HOH | | 30 | 46.444 | 34.888 | -14.485 | 1.00 | 30.70 | |
| ATOM | 1952 | O | HOH | | 31 | 42.905 | 22.704 | -2.761 | 1.00 | 21.06 | |
| ATOM | 1953 | O | HOH | | 32 | 45.201 | 36.882 | -11.552 | 1.00 | 28.24 | |
| ATOM | 1954 | O | HOH | | 33 | 25.649 | 19.886 | 8.886 | 1.00 | 28.23 | |
| ATOM | 1955 | O | HOH | | 34 | 26.045 | 10.696 | 12.207 | 1.00 | 26.17 | |
| ATOM | 1956 | O | HOH | | 35 | 32.469 | 36.471 | 23.268 | 1.00 | 30.94 | |
| ATOM | 1957 | O | HOH | | 36 | 45.943 | 28.640 | 19.548 | 1.00 | 23.84 | |
| ATOM | 1958 | O | HOH | | 37 | 43.494 | 30.640 | -16.264 | 1.00 | 19.57 | |
| ATOM | 1959 | O | HOH | | 38 | 40.052 | 27.988 | 21.059 | 1.00 | 19.96 | |
| ATOM | 1960 | O | HOH | | 39 | 30.163 | 11.427 | -5.817 | 1.00 | 23.16 | |
| ATOM | 1961 | O | HOH | | 40 | 22.655 | 26.060 | -1.019 | 1.00 | 25.88 | |
| ATOM | 1962 | O | HOH | | 41 | 47.443 | 25.123 | -1.056 | 1.00 | 26.06 | |
| ATOM | 1963 | O | HOH | | 42 | 43.351 | 38.717 | -10.710 | 1.00 | 31.36 | |
| ATOM | 1964 | O | HOH | | 43 | 47.439 | 22.148 | 9.534 | 1.00 | 23.85 | |
| ATOM | 1965 | O | HOH | | 44 | 39.265 | 8.211 | 3.837 | 1.00 | 24.72 | |
| ATOM | 1966 | O | HOH | | 45 | 29.442 | 47.107 | 13.465 | 1.00 | 28.59 | |
| ATOM | 1967 | O | HOH | | 46 | 49.276 | 48.894 | -1.723 | 1.00 | 23.41 | |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1968 | O | HOH | 47 | 36.013 | 33.810 | 24.513 | 1.00 | 26.17 |
| ATOM | 1969 | O | HOH | 48 | 41.724 | 36.316 | 13.254 | 1.00 | 25.30 |
| ATOM | 1970 | O | HOH | 49 | 38.645 | 15.363 | -8.356 | 1.00 | 24.55 |
| ATOM | 1971 | O | HOH | 50 | 31.955 | 12.217 | 13.710 | 1.00 | 26.51 |
| ATOM | 1972 | O | HOH | 51 | 45.068 | 55.619 | 1.338 | 1.00 | 27.50 |
| ATOM | 1973 | O | HOH | 52 | 43.052 | 19.153 | 9.777 | 1.00 | 23.61 |
| ATOM | 1974 | O | HOH | 53 | 45.777 | 32.997 | -12.641 | 1.00 | 28.74 |
| ATOM | 1975 | O | HOH | 54 | 28.793 | 15.549 | -7.585 | 1.00 | 26.71 |
| ATOM | 1976 | O | HOH | 55 | 49.821 | 42.639 | -12.216 | 1.00 | 30.32 |
| ATOM | 1977 | O | HOH | 56 | 21.473 | 35.733 | -4.098 | 1.00 | 21.73 |
| ATOM | 1978 | O | HOH | 57 | 42.925 | 18.920 | -.016 | 1.00 | 30.56 |
| ATOM | 1979 | O | HOH | 58 | 28.680 | -.098 | 15.206 | 1.00 | 24.41 |
| ATOM | 1980 | O | HOH | 59 | 30.575 | 22.738 | 24.395 | 1.00 | 28.00 |
| ATOM | 1981 | O | HOH | 60 | 17.766 | 10.990 | 3.488 | 1.00 | 31.85 |
| ATOM | 1982 | O | HOH | 61 | 49.649 | 49.378 | -5.610 | 1.00 | 38.05 |
| ATOM | 1983 | O | HOH | 62 | 47.518 | 52.219 | -2.812 | 1.00 | 26.66 |
| ATOM | 1984 | O | HOH | 63 | 41.787 | 11.851 | 9.383 | 1.00 | 31.75 |
| ATOM | 1985 | O | HOH | 64 | 19.342 | 13.836 | 4.361 | 1.00 | 26.81 |
| ATOM | 1986 | O | HOH | 65 | 28.428 | 11.606 | 12.742 | 1.00 | 32.86 |
| ATOM | 1987 | O | HOH | 66 | 26.186 | 41.935 | .560 | 1.00 | 29.32 |
| ATOM | 1988 | O | HOH | 67 | 29.916 | 3.091 | 12.731 | 1.00 | 35.96 |
| ATOM | 1989 | O | HOH | 68 | 32.525 | 39.422 | -19.919 | 1.00 | 28.79 |
| ATOM | 1990 | O | HOH | 69 | 23.391 | 12.991 | -5.165 | 1.00 | 27.70 |
| ATOM | 1991 | O | HOH | 70 | 37.988 | 45.231 | 8.061 | 1.00 | 31.23 |
| ATOM | 1992 | O | HOH | 71 | 51.112 | 27.635 | -9.569 | 1.00 | 27.13 |
| ATOM | 1993 | O | HOH | 72 | 44.253 | 30.674 | -13.637 | 1.00 | 26.48 |
| ATOM | 1994 | O | HOH | 73 | 50.881 | 30.964 | -3.729 | 1.00 | 34.82 |
| ATOM | 1995 | O | HOH | 74 | 40.933 | 28.825 | -10.989 | 1.00 | 42.43 |
| ATOM | 1996 | O | HOH | 75 | 27.184 | 22.223 | 9.119 | 1.00 | 27.88 |
| ATOM | 1997 | O | HOH | 76 | 34.540 | 39.110 | 11.358 | 1.00 | 40.78 |
| ATOM | 1998 | O | HOH | 77 | 46.502 | 22.169 | -3.457 | 1.00 | 30.26 |
| ATOM | 1999 | O | HOH | 78 | 53.219 | 46.329 | -17.171 | 1.00 | 28.75 |
| ATOM | 2000 | O | HOH | 79 | 26.474 | 24.441 | -5.560 | 1.00 | 27.23 |
| ATOM | 2001 | O | HOH | 80 | 21.166 | 23.641 | -4.948 | 1.00 | 35.36 |
| ATOM | 2002 | O | HOH | 81 | 46.816 | 32.597 | 16.414 | 1.00 | 35.59 |
| ATOM | 2003 | O | HOH | 82 | 29.879 | 14.101 | 14.638 | 1.00 | 31.68 |
| ATOM | 2004 | O | HOH | 83 | 21.692 | 33.500 | 2.984 | 1.00 | 30.16 |
| ATOM | 2005 | O | HOH | 84 | 29.295 | 27.121 | 22.187 | 1.00 | 25.57 |
| ATOM | 2006 | O | HOH | 85 | 28.731 | 12.779 | -8.089 | 1.00 | 38.33 |
| ATOM | 2007 | O | HOH | 86 | 27.280 | 16.834 | -9.400 | 1.00 | 46.09 |
| ATOM | 2008 | O | HOH | 87 | 26.071 | 25.682 | -7.687 | 1.00 | 35.23 |
| ATOM | 2009 | O | HOH | 88 | 31.705 | 45.557 | 4.386 | 1.00 | 36.53 |
| ATOM | 2010 | O | HOH | 89 | 42.737 | 27.677 | -16.494 | 1.00 | 43.50 |
| ATOM | 2011 | O | HOH | 90 | 35.195 | 13.995 | 13.837 | 1.00 | 34.72 |
| ATOM | 2012 | O | HOH | 91 | 49.946 | 45.582 | -18.866 | 1.00 | 29.05 |
| ATOM | 2013 | O | HOH | 92 | 49.674 | 15.137 | 4.173 | 1.00 | 42.43 |
| ATOM | 2014 | O | HOH | 93 | 24.992 | 40.863 | 2.394 | 1.00 | 29.44 |
| ATOM | 2015 | O | HOH | 94 | 35.938 | 29.931 | 22.590 | 1.00 | 33.47 |
| ATOM | 2016 | O | HOH | 95 | 36.358 | 31.790 | 18.073 | 1.00 | 38.64 |
| ATOM | 2017 | O | HOH | 96 | 47.419 | 54.724 | -3.794 | 1.00 | 29.22 |
| ATOM | 2018 | O | HOH | 97 | 47.298 | 25.185 | -13.959 | 1.00 | 27.59 |
| ATOM | 2019 | O | HOH | 98 | 49.410 | 31.445 | -.598 | 1.00 | 37.89 |
| ATOM | 2020 | O | HOH | 99 | 32.034 | 44.105 | -10.298 | 1.00 | 32.29 |
| ATOM | 2021 | O | HOH | 100 | 46.589 | 20.057 | 12.718 | 1.00 | 35.82 |
| ATOM | 2022 | O | HOH | 101 | 40.404 | 18.582 | 19.335 | 1.00 | 37.38 |
| ATOM | 2023 | O | HOH | 102 | 36.397 | 37.290 | 23.171 | 1.00 | 38.30 |
| ATOM | 2024 | O | HOH | 103 | 45.419 | 35.806 | 6.232 | 1.00 | 39.97 |
| ATOM | 2025 | O | HOH | 104 | 39.400 | 18.431 | 15.599 | 1.00 | 28.80 |
| ATOM | 2026 | O | HOH | 105 | 32.747 | 22.249 | 25.771 | 1.00 | 35.21 |
| ATOM | 2027 | O | HOH | 106 | 31.993 | 43.225 | -12.811 | 1.00 | 31.67 |
| ATOM | 2028 | O | HOH | 107 | 36.965 | 41.556 | 8.934 | 1.00 | 34.98 |
| ATOM | 2029 | O | HOH | 108 | 28.311 | 37.534 | 18.638 | 1.00 | 41.87 |
| ATOM | 2030 | O | HOH | 109 | 43.152 | 40.996 | -17.014 | 1.00 | 34.31 |
| ATOM | 2031 | O | HOH | 110 | 36.900 | 23.769 | 24.433 | 1.00 | 36.25 |
| ATOM | 2032 | O | HOH | 111 | 22.163 | 15.646 | 14.398 | 1.00 | 36.85 |
| ATOM | 2033 | O | HOH | 112 | 35.492 | 21.090 | 24.155 | 1.00 | 42.67 |
| ATOM | 2034 | O | HOH | 113 | 48.632 | 28.953 | 2.985 | 1.00 | 31.18 |
| ATOM | 2035 | O | HOH | 114 | 39.959 | 28.401 | -13.559 | 1.00 | 38.45 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2036 | O | HOH | 115 | 32.211 | 44.343 | 12.977 | 1.00 | 35.11 |
| ATOM | 2037 | O | HOH | 116 | 57.018 | 43.358 | -20.359 | 1.00 | 34.09 |
| ATOM | 2038 | O | HOH | 117 | 43.928 | 36.491 | 15.046 | 1.00 | 44.76 |
| ATOM | 2039 | O | HOH | 118 | 41.009 | 17.495 | -8.021 | 1.00 | 28.89 |
| ATOM | 2040 | O | HOH | 119 | 47.866 | 53.440 | 6.326 | 1.00 | 43.86 |
| ATOM | 2041 | O | HOH | 120 | 19.063 | 32.664 | 8.432 | 1.00 | 51.10 |
| ATOM | 2042 | O | HOH | 121 | 35.431 | 41.465 | 11.175 | 1.00 | 35.75 |
| ATOM | 2043 | O | HOH | 122 | 41.401 | 44.934 | -4.130 | 1.00 | 32.52 |
| ATOM | 2044 | O | HOH | 123 | 43.399 | 15.096 | -1.902 | 1.00 | 35.28 |
| ATOM | 2045 | O | HOH | 124 | 50.234 | 39.780 | -12.613 | 1.00 | 40.18 |
| ATOM | 2046 | O | HOH | 125 | 43.037 | 30.072 | 18.750 | 1.00 | 45.64 |
| ATOM | 2047 | O | HOH | 126 | 44.652 | 33.989 | 15.169 | 1.00 | 36.16 |
| ATOM | 2048 | O | HOH | 127 | 38.229 | 48.920 | 9.835 | 1.00 | 47.09 |
| ATOM | 2049 | O | HOH | 128 | 44.947 | 18.550 | 19.997 | 1.00 | 36.95 |
| ATOM | 2050 | O | HOH | 129 | 19.249 | 33.307 | -4.291 | 1.00 | 35.52 |
| ATOM | 2051 | O | HOH | 130 | 20.932 | 42.677 | 5.492 | 1.00 | 38.75 |
| ATOM | 2052 | O | HOH | 131 | 32.240 | 5.674 | -7.678 | 1.00 | 42.41 |
| ATOM | 2053 | O | HOH | 132 | 25.079 | 5.184 | 2.319 | 1.00 | 43.83 |
| ATOM | 2054 | O | HOH | 133 | 47.452 | 34.447 | -8.833 | 1.00 | 33.02 |
| ATOM | 2055 | O | HOH | 134 | 31.823 | 25.421 | -14.083 | 1.00 | 43.26 |
| ATOM | 2056 | O | HOH | 135 | 21.662 | 1.721 | 13.249 | 1.00 | 37.77 |
| ATOM | 2057 | O | HOH | 136 | 43.284 | 20.715 | -10.461 | 1.00 | 32.13 |
| ATOM | 2058 | O | HOH | 137 | 23.845 | 9.069 | -4.875 | 1.00 | 37.96 |
| ATOM | 2059 | O | HOH | 138 | 42.205 | 23.336 | -17.516 | 1.00 | 39.25 |
| ATOM | 2060 | O | HOH | 139 | 23.782 | 47.257 | 8.875 | 1.00 | 36.18 |
| ATOM | 2061 | O | HOH | 140 | 40.071 | 29.109 | 18.652 | 1.00 | 36.37 |
| ATOM | 2062 | O | HOH | 141 | 50.037 | 23.125 | 9.649 | 1.00 | 45.98 |
| ATOM | 2063 | O | HOH | 142 | 19.583 | 34.873 | 10.411 | 1.00 | 47.78 |
| ATOM | 2064 | O | HOH | 143 | 43.464 | 17.607 | 18.095 | 1.00 | 47.57 |
| ATOM | 2065 | O | HOH | 144 | 25.361 | 15.356 | 16.333 | 1.00 | 41.25 |
| ATOM | 2066 | O | HOH | 145 | 28.757 | 38.927 | -17.342 | 1.00 | 34.49 |
| ATOM | 2067 | O | HOH | 146 | 23.938 | -1.305 | 12.858 | 1.00 | 51.98 |
| ATOM | 2068 | O | HOH | 147 | 33.517 | 18.774 | -13.399 | 1.00 | 46.54 |
| ATOM | 2069 | O | HOH | 148 | 49.091 | 33.188 | 18.209 | 1.00 | 46.77 |
| ATOM | 2070 | O | HOH | 149 | 50.357 | 27.234 | -.902 | 1.00 | 40.05 |
| ATOM | 2071 | O | HOH | 150 | 25.608 | 6.521 | -2.912 | 1.00 | 43.02 |
| ATOM | 2072 | O | HOH | 151 | 38.264 | 4.869 | -2.160 | 1.00 | 38.27 |
| ATOM | 2073 | O | HOH | 152 | 62.716 | 38.725 | -15.633 | 1.00 | 47.64 |
| ATOM | 2074 | O | HOH | 153 | 47.852 | 13.446 | 6.230 | 1.00 | 45.10 |
| ATOM | 2075 | O | HOH | 154 | 30.371 | 42.873 | -21.841 | 1.00 | 49.83 |
| ATOM | 2076 | O | HOH | 155 | 25.807 | 26.178 | -10.206 | 1.00 | 41.92 |
| ATOM | 2077 | O | HOH | 156 | 20.377 | 17.443 | -2.962 | 1.00 | 37.23 |
| ATOM | 2078 | O | HOH | 157 | 26.310 | 19.158 | -9.197 | 1.00 | 40.75 |
| ATOM | 2079 | O | HOH | 158 | 44.764 | 43.862 | -15.074 | 1.00 | 46.84 |
| ATOM | 2080 | O | HOH | 159 | 38.089 | 28.511 | 23.290 | 1.00 | 52.16 |
| ATOM | 2081 | O | HOH | 160 | 39.671 | 34.256 | 14.970 | 1.00 | 52.34 |
| ATOM | 2082 | O | HOH | 161 | 20.912 | 34.446 | 6.722 | 1.00 | 51.80 |
| ATOM | 2083 | O | HOH | 162 | 47.355 | 17.692 | 16.464 | 1.00 | 44.35 |
| ATOM | 2084 | O | HOH | 163 | 40.877 | 24.164 | -19.590 | 1.00 | 50.62 |
| ATOM | 2085 | O | HOH | 164 | 22.739 | 41.807 | 2.902 | 1.00 | 45.77 |
| ATOM | 2086 | O | HOH | 165 | 19.295 | 40.596 | -6.896 | 1.00 | 40.71 |
| ATOM | 2087 | O | HOH | 166 | 44.688 | 45.877 | 11.462 | 1.00 | 49.75 |
| ATOM | 2088 | O | HOH | 167 | 65.941 | 38.623 | -21.101 | 1.00 | 41.18 |
| ATOM | 2089 | O | HOH | 168 | 20.892 | 37.818 | 3.324 | 1.00 | 36.26 |
| ATOM | 2090 | O | HOH | 169 | 23.791 | 54.770 | -.960 | 1.00 | 47.88 |
| ATOM | 2091 | O | HOH | 170 | 37.603 | 28.849 | -15.685 | 1.00 | 40.98 |
| ATOM | 2092 | O | HOH | 171 | 45.555 | 18.839 | .687 | 1.00 | 36.06 |
| ATOM | 2093 | O | HOH | 172 | 35.456 | 41.167 | -13.948 | 1.00 | 25.05 |
| ATOM | 2094 | O | HOH | 173 | 31.200 | 38.910 | -25.308 | 1.00 | 37.28 |
| ATOM | 2095 | O | HOH | 174 | 21.554 | 13.921 | 10.766 | 1.00 | 36.99 |
| ATOM | 2096 | O | HOH | 175 | 46.026 | 26.992 | -15.385 | 1.00 | 39.58 |
| ATOM | 2097 | O | HOH | 176 | 37.903 | 17.801 | 18.592 | 1.00 | 48.95 |
| ATOM | 2098 | O | HOH | 177 | 43.747 | 13.395 | 8.035 | 1.00 | 39.48 |
| ATOM | 2099 | O | HOH | 178 | 34.071 | 38.400 | 19.794 | 1.00 | 35.56 |
| ATOM | 2100 | O | HOH | 179 | 43.250 | 39.476 | 13.165 | 1.00 | 37.82 |
| ATOM | 2101 | O | HOH | 180 | 41.483 | 7.783 | 2.019 | 1.00 | 45.02 |
| ATOM | 2102 | O | HOH | 181 | 65.389 | 34.398 | -23.115 | 1.00 | 42.44 |
| ATOM | 2103 | O | HOH | 182 | 33.931 | 41.093 | 14.772 | 1.00 | 41.75 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2104 | O | HOH | 183 | 20.394 | 26.531 | -2.994 | 1.00 | 45.01 |
| ATOM | 2105 | O | HOH | 184 | 46.284 | 41.009 | 9.919 | 1.00 | 41.10 |
| ATOM | 2106 | O | HOH | 185 | 47.034 | 40.049 | -9.804 | 1.00 | 36.98 |
| ATOM | 2107 | O | HOH | 186 | 49.956 | 29.227 | .659 | 1.00 | 41.68 |
| ATOM | 2108 | O | HOH | 187 | 25.126 | 33.755 | 20.531 | 1.00 | 45.06 |
| ATOM | 2109 | O | HOH | 188 | 45.660 | 12.088 | 6.545 | 1.00 | 47.03 |
| ATOM | 2110 | O | HOH | 189 | 53.064 | 31.023 | -2.009 | 1.00 | 44.55 |
| ATOM | 2111 | O | HOH | 190 | 21.902 | 54.378 | -2.782 | 1.00 | 45.52 |
| ATOM | 2112 | O | HOH | 191 | 47.488 | 40.412 | 5.641 | 1.00 | 38.47 |
| ATOM | 2113 | O | HOH | 192 | 23.372 | 38.108 | -12.261 | 1.00 | 36.78 |
| ATOM | 2114 | O | HOH | 193 | 32.823 | 6.238 | 8.957 | 1.00 | 31.69 |
| ATOM | 2115 | O | HOH | 194 | 21.776 | 33.149 | 15.893 | 1.00 | 43.71 |
| ATOM | 2116 | O | HOH | 195 | 25.948 | 2.717 | 3.211 | 1.00 | 41.21 |
| ATOM | 2117 | O | HOH | 196 | 37.457 | 24.842 | -16.507 | 1.00 | 48.71 |
| ATOM | 2118 | O | HOH | 197 | 25.655 | 4.669 | -.498 | 1.00 | 41.01 |
| ATOM | 2119 | O | HOH | 198 | 34.993 | 41.490 | -16.488 | 1.00 | 42.97 |
| ATOM | 2120 | O | HOH | 199 | 51.572 | 32.788 | -1.315 | 1.00 | 41.87 |
| ATOM | 2121 | O | HOH | 200 | 34.147 | 30.225 | -17.326 | 1.00 | 37.43 |
| ATOM | 2122 | O | HOH | 201 | 55.135 | 44.572 | -21.602 | 1.00 | 41.06 |
| ATOM | 2123 | O | HOH | 202 | 25.757 | 45.671 | -7.830 | 1.00 | 44.53 |
| ATOM | 2124 | O | HOH | 203 | 37.549 | 6.250 | 2.375 | 1.00 | 38.07 |
| ATOM | 2125 | O | HOH | 204 | 16.646 | 31.917 | 2.952 | 1.00 | 42.39 |
| ATOM | 2126 | O | HOH | 205 | 49.733 | 40.229 | 1.785 | 1.00 | 43.85 |
| ATOM | 2127 | O | HOH | 206 | 46.253 | 39.703 | 7.766 | 1.00 | 42.68 |
| ATOM | 2128 | O | HOH | 207 | 37.677 | 35.948 | 18.903 | 1.00 | 45.70 |
| ATOM | 2129 | O | HOH | 208 | 23.633 | 36.693 | 17.352 | 1.00 | 40.00 |
| ATOM | 2130 | O | HOH | 209 | 54.776 | 29.648 | 2.106 | 1.00 | 45.43 |
| ATOM | 2131 | O | HOH | 210 | 27.204 | 25.113 | -13.388 | 1.00 | 42.37 |
| ATOM | 2132 | O | HOH | 211 | 16.997 | 29.300 | -.454 | 1.00 | 42.78 |
| ATOM | 2133 | O | HOH | 212 | 44.578 | 21.178 | -4.267 | 1.00 | 45.11 |
| ATOM | 2134 | O | HOH | 213 | 34.450 | 39.857 | -18.339 | 1.00 | 40.15 |
| ATOM | 2135 | O | HOH | 214 | 48.993 | 29.855 | -2.640 | 1.00 | 48.30 |
| ATOM | 2136 | O | HOH | 215 | 47.166 | 30.914 | 6.435 | 1.00 | 40.03 |
| ATOM | 2137 | O | HOH | 216 | 24.477 | 38.679 | 9.302 | 1.00 | 44.85 |
| ATOM | 2138 | O | HOH | 217 | 40.570 | 31.936 | 15.567 | 1.00 | 39.55 |
| ATOM | 2139 | O | HOH | 218 | 47.679 | 19.437 | 9.176 | 1.00 | 46.30 |
| ATOM | 2140 | O | HOH | 219 | 49.467 | 32.411 | 20.725 | 1.00 | 49.57 |
| ATOM | 2141 | O | HOH | 220 | 40.564 | 48.980 | -8.727 | 1.00 | 38.53 |
| ATOM | 2142 | O | HOH | 221 | 51.817 | 27.969 | 14.989 | 1.00 | 45.36 |
| ATOM | 2143 | O | HOH | 222 | 45.303 | 19.657 | 10.595 | 1.00 | 50.38 |
| ATOM | 2144 | O | HOH | 223 | 37.514 | 51.784 | 9.970 | 1.00 | 45.01 |
| ATOM | 2145 | O | HOH | 224 | 23.691 | 17.281 | -6.725 | 1.00 | 34.27 |
| ATOM | 2146 | O | HOH | 225 | 39.832 | 6.213 | -.004 | 1.00 | 43.18 |
| ATOM | 2147 | O | HOH | 226 | 14.435 | 31.992 | 6.539 | 1.00 | 40.54 |
| ATOM | 2148 | O | HOH | 227 | 28.440 | 3.081 | -.375 | 1.00 | 40.66 |
| ATOM | 2149 | O | HOH | 228 | 32.185 | 1.604 | -.032 | 1.00 | 39.88 |
| ATOM | 2150 | O | HOH | 229 | 31.504 | 47.620 | 2.802 | 1.00 | 38.71 |
| ATOM | 2151 | O | HOH | 230 | 43.339 | 48.665 | -10.895 | 1.00 | 40.50 |
| ATOM | 2152 | O | HOH | 231 | 48.992 | 42.900 | -8.868 | 1.00 | 40.18 |
| ATOM | 2153 | O | HOH | 232 | 50.311 | 46.431 | -10.063 | 1.00 | 38.69 |
| ATOM | 2154 | O | HOH | 233 | 45.885 | 49.961 | -12.873 | 1.00 | 42.42 |
| ATOM | 2155 | O | HOH | 234 | 21.172 | 36.234 | 8.566 | 1.00 | 42.66 |
| ATOM | 2156 | O | HOH | 235 | 19.309 | 10.393 | 10.198 | 1.00 | 38.58 |
| ATOM | 2157 | O | HOH | 236 | 35.310 | 7.159 | 11.114 | 1.00 | 38.88 |
| ATOM | 2158 | O | HOH | 237 | 48.544 | 43.963 | 6.735 | 1.00 | 41.80 |
| ATOM | 2159 | O | HOH | 238 | 37.971 | 55.166 | 6.733 | 1.00 | 39.07 |
| ATOM | 2160 | O | HOH | 239 | 32.689 | 38.646 | 24.608 | 1.00 | 39.11 |
| ATOM | 2161 | O | HOH | 240 | 36.473 | 38.193 | 18.321 | 1.00 | 41.71 |
| ATOM | 2162 | O | HOH | 241 | 25.507 | 41.267 | -12.919 | 1.00 | 35.13 |
| ATOM | 2163 | O | HOH | 242 | 23.143 | 35.618 | -15.172 | 1.00 | 39.82 |
| ATOM | 2164 | O | HOH | 243 | 49.140 | 33.897 | 5.783 | 1.00 | 40.42 |
| ATOM | 2165 | O | HOH | 244 | 29.532 | 27.579 | -16.268 | 1.00 | 39.77 |
| ATOM | 2166 | O | HOH | 245 | 26.507 | 50.321 | 5.926 | 1.00 | 35.74 |
| ATOM | 2167 | O | HOH | 246 | 24.886 | 49.944 | 8.651 | 1.00 | 37.76 |
| ATOM | 2168 | O | HOH | 247 | 33.171 | 50.567 | 6.460 | 1.00 | 35.10 |
| ATOM | 2169 | C1 | EDO | 1 | 49.678 | 27.876 | 17.913 | 1.00 | 32.33 |
| ATOM | 2170 | O1 | EDO | 1 | 48.324 | 27.636 | 18.334 | 1.00 | 32.24 |
| ATOM | 2171 | C2 | EDO | 1 | 49.859 | 29.331 | 17.617 | 1.00 | 33.08 |

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ATOM   2172  O2  EDO     1      49.776  29.707  16.203  1.00 33.95
ATOM   2173  C1  EDO     2      35.821  26.057 -12.559  1.00 27.36
ATOM   2174  O1  EDO     2      35.083  24.825 -12.633  1.00 26.99
ATOM   2175  C2  EDO     2      37.288  25.766 -12.507  1.00 27.04
ATOM   2176  O2  EDO     2      37.823  25.421 -11.188  1.00 26.81
ATOM   2177  C1  EDO     3      32.109   4.707  -1.196  1.00 32.05
ATOM   2178  O1  EDO     3      30.999   3.924   -.720  1.00 34.90
ATOM   2179  C2  EDO     3      32.483   5.724   -.166  1.00 30.33
ATOM   2180  O2  EDO     3      33.342   5.246    .915  1.00 32.01
ATOM   2181  C1  EDO     4      20.413  30.402  -8.539  1.00 38.13
ATOM   2182  O1  EDO     4      20.666  29.723  -7.292  1.00 38.27
ATOM   2183  C2  EDO     4      20.600  31.879  -8.368  1.00 38.37
ATOM   2184  O2  EDO     4      20.800  32.350  -6.995  1.00 38.66
ATOM   2185  C1  EDO     5      21.662  24.418   7.348  1.00 35.45
ATOM   2186  O1  EDO     5      23.030  24.437   7.797  1.00 36.25
ATOM   2187  C2  EDO     5      21.624  24.463   5.852  1.00 35.50
ATOM   2188  O2  EDO     5      21.767  25.789   5.249  1.00 36.44
ATOM   2189 MG+2 MG2    1      43.852  18.841   2.109  1.00 27.78
ATOM   2190 CL-1 CL1    1      24.304  20.875   1.803  1.00 17.97
ATOM   2191  N   MSE   158      35.110  34.014   5.907   .44 10.21      AC2
ATOM   2192  CA  MSE   158      34.354  34.920   5.054   .44 11.98      AC2
ATOM   2193  CB  MSE   158      35.299  35.639   4.091   .44 15.25      AC2
ATOM   2194  CG  MSE   158      34.663  36.759   3.292   .44 19.01      AC2
ATOM   2195  SE  MSE   158      35.246  38.493   3.909   .44 26.38      AC2
ATOM   2196  CE  MSE   158      37.144  38.257   3.682   .44 20.56      AC2
ATOM   2197  C   MSE   158      33.395  34.019   4.277   .44 11.27      AC2
ATOM   2198  O   MSE   158      33.821  33.037   3.669   .44 11.23      AC2
ATOM   2199  N   SER   208      39.368  41.606   .024   .50  5.19      AC2
ATOM   2200  CA  SER   208      40.803  41.859   .059   .50  6.96      AC2
ATOM   2201  CB  SER   208      41.287  42.307  -1.316   .50  6.77      AC2
ATOM   2202  OG  SER   208      41.093  41.278  -2.266   .50 12.86      AC2
ATOM   2203  C   SER   208      41.172  42.904   1.102   .50  5.34      AC2
ATOM   2204  O   SER   208      42.168  42.759   1.808   .50  2.94      AC2
ATOM   2205  N   ILE   220      34.627  31.400   1.641   .50  1.35      AC2
ATOM   2206  CA  ILE   220      33.627  30.506   1.061   .50  1.35      AC2
ATOM   2207  CB  ILE   220      32.618  30.008   2.134   .50  1.35      AC2
ATOM   2208  CG2 ILE   220      31.422  29.326   1.458   .50  1.35      AC2
ATOM   2209  CG1 ILE   220      33.312  29.085   3.141   .50  1.97      AC2
ATOM   2210  CD1 ILE   220      33.863  27.818   2.556   .50  8.09      AC2
ATOM   2211  C   ILE   220      32.807  31.257   .020   .50  1.35      AC2
ATOM   2212  O   ILE   220      32.421  32.406   .246   .50  1.35      AC2
ATOM   2213  N   MSE   326      33.175   8.443   2.911   .39 17.50      AC2
ATOM   2214  CA  MSE   326      31.818   8.709   3.360   .39 17.68      AC2
ATOM   2215  CB  MSE   326      31.105   7.414   3.748   .39 21.36      AC2
ATOM   2216  CG  MSE   326      30.708   6.543   2.581   .39 24.62      AC2
ATOM   2217  SE  MSE   326      29.821   4.948   3.175   .39 34.10      AC2
ATOM   2218  CE  MSE   326      27.998   5.567   3.081   .39 30.04      AC2
ATOM   2219  C   MSE   326      31.873   9.621   4.568   .39 16.52      AC2
ATOM   2220  O   MSE   326      32.839   9.602   5.331   .39 17.10      AC2
ATOM   2221  CB  PRO  1519      23.711  50.412   .520   .50 37.35      AC2
ATOM   2222  CG  PRO  1519      24.961  50.755  -.261   .50 38.95      AC2
ATOM   2223  C   PRO  1519      24.595  49.927  2.807   .50 36.73      AC2
ATOM   2224  O   PRO  1519      25.750  49.985  3.197   .50 37.75      AC2
ATOM   2225  N   PRO  1519      25.010  52.092  1.661   .50 38.05      AC2
ATOM   2226  CD  PRO  1519      25.361  52.159   .229   .50 38.46      AC2
ATOM   2227  CA  PRO  1519      24.029  50.997  1.887   .50 37.02      AC2
END
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FIGURE 2

Table 2 **Crystallographic data on the BRC4-RAD51 complex.**

Diffraction data (space group: $P2_12_12_1$: *a*=57.30Å, *b*=59.14Å, *c*=77.20Å)

| Dataset | Resolution | Wavelength | Reflections[1] (unique) | Completeness (outer shell) | $R_{sym}$[2] (outer shell) | I/σ(I) | Beamline |
|---|---|---|---|---|---|---|---|
| Native | 1.8Å | 1.5418Å | 169388 (24702) | 99.9 (99.1) | 0.051 (0.308) | 40.9 (6.7) | In-house |
| $KAu(CN)_2$ | 2.0Å | 1.5418Å | 179758 (18077) | 100.0 (100.0) | 0.059 (0.194) | 36.6 (11.9) | In-house |
| SeMet, peak | 1.7Å | 0.9792Å | 204230 (29143) | 99.9 (99.9) | 0.077 (0.321) | 23.5 (6.5) | ESRF, ID-29 |
| SeMet, remote | 1.7Å | 0.90831Å | 207259 (29329) | 99.9 (99.6) | 0.070 (0.481) | 24.7 (4.2) | ESRF, ID-29 |

Phasing

| | $KAu(CN)_2$ | SeMet, peak | SeMet, remote |
|---|---|---|---|
| Rcullis (iso/ano)[3] | 0.93 / 0.95 | - , 0.70 | 0.84 / 0.84 |
| Phasing power (iso/ano)[4] | 0.72 / 0.74 | - , 2.1 | 0.48 / 1.65 |
| Figure of merit[5] | 0.21 | 0.51 | |

Refinement[6]

| Resolution (Å) | Reflections | Number of non-H atoms | R[7] (%) | $R_{free}$ (%) | <B> ($A^2$) | Rmsd bonds (Å) | Rmsd angles (°) |
|---|---|---|---|---|---|---|---|
| 24.8-1.7 | 55746 | 2179 | 19.1 | 20.6 | 21.1 | 0.006 | 1.229 |

[1] For MAD data, the Bijvoet pairs were not merged.

[2] $R_{sym} = \sum_{hkl}\sum_{i}\left|I_i(hkl) - \langle I_i(hkl)\rangle\right| \Big/ \sum_{hkl}\sum_{i} I_i(hkl)$

[3] $R_{cullis}$ as defined in SHARP.

[4] Phasing power as defined in SHARP.

[5] Figure of merit as defined in SHARP.

[6] Statistics for all data.

[7] R-factor $= \sum_{hkl}\left|\,|F_{obs}| - |F_{calc}|\,\right| \Big/ \sum_{hkl}|F_{obs}|$

FIGURE 3

Table 3 **Structure-based analysis of BRCA2 BRC sequence conservation.**

| | | | | β | β | β | | | | β | β | β | | | | α | α | α | α | α | α | α | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | L | L | G | F | H | T | A | S | G | K | K | V | K | I | A | K | E | S | L | D | K | V | K | N | L | F | D | E |
| D | 2 | | | | 1 | | 2 | 3 | | 1 | | | | | | 8 | 1 | | | 6 | 2 | 2 | | 1 | 2 | 1 | 8 | 17 |
| E | 1 | 1 | | | | | 1 | | 1 | 1 | 9 | | 2 | | | 21 | 22 | | | 3 | 4 | 1 | 1 | 4 | | | 7 | 28 |
| K | 1 | | 1 | | 1 | | | 1 | | 39 | 20 | | 12 | 1 | | 10 | 2 | | 1 | 8 | 44 | | 27 | 12 | 2 | 1 | 9 | 1 |
| R | | 4 | | 1 | 8 | | | 1 | 1 | 5 | 2 | | 4 | 2 | 1 | 2 | | | | 4 | 1 | | 11 | 1 | 1 | | 6 | 1 |
| H | | | | | 6 | | | 6 | 1 | | | | | | | 3 | 4 | | | 5 | | 1 | | | | | | |
| N | 3 | 1 | 1 | | | | | 1 | 7 | | 7 | 1 | 4 | | | 2 | 1 | 6 | | 5 | 1 | 2 | 1 | 11 | | | 5 | |
| Q | | 1 | | 1 | 8 | 1 | | | | 3 | 5 | | 7 | | | 5 | 1 | | | 8 | | | | 8 | | | 1 | 4 |
| S | 3 | 7 | 12 | | 17 | 7 | 2 | 33 | 8 | | 3 | | 13 | | 39 | 2 | 13 | 28 | | 4 | 2 | 11 | | 3 | | | 14 | |
| T | | 2 | 2 | | 2 | 45 | 1 | 1 | 1 | 5 | | 8 | 5 | | 5 | 2 | 3 | 3 | | 3 | 2 | | | | 1 | | 3 | 1 |
| G | 5 | 15 | 21 | | | | 2 | 4 | 37 | 1 | | | | | 2 | | 1 | | | | | 3 | 1 | 6 | | | | |
| A | 6 | | 7 | | | 1 | 46 | | | | 5 | | | | 4 | | 8 | 15 | | 3 | | 19 | 1 | 1 | | | 1 | |
| P | 5 | 4 | | | | | 1 | | | | 1 | | 1 | | | | | | | | | | | | | | | 1 |
| C | 3 | | | 2 | 3 | | | 2 | | | | 1 | 5 | | | | | | | 1 | | 2 | | | | | | 1 |
| I | | 4 | 5 | | 3 | 1 | | | | 2 | 16 | | 12 | | | | 2 | 8 | | | 3 | | | 6 | 2 | | 1 |
| L | 8 | 16 | | | | 1 | | 3 | | 2 | 6 | | 7 | 1 | | | 1 | 38 | 3 | | | 1 | | 17 | 17 | | | |
| V | 2 | 1 | 4 | | | | 1 | 1 | | 1 | | 23 | 2 | 33 | | 1 | | 4 | 1 | | 14 | 7 | | 7 | | 2 | 1 |
| M | | | | | | | | | | | | | | | 4 | | | | | | | 4 | 7 | 6 | | | | |
| F | 14 | | 3 | 50 | | | | | | | | 1 | 1 | 1 | | | 1 | 4 | 2 | | | | 1 | 8 | 35 | | | |
| W | | | | | | | | | | | | | | | | | | | | | | | | 6 | | | | |
| Y | 3 | | | 2 | 7 | | | | | | | | | | | | | 1 | | | | | 1 | | | | | |

Consensus:

| | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | G | F | *x* | T | A | S | G | K | *o* | *i* | *x* | *i* | S | *o* | *o* | S | L | *x* | K | A | K | *x* | *i* | F | *o* | D |
| | S | | | S | | | S | | | | | | | | | A | | | | V | R | | *a* | L | | E |
| | | | | | | | N | | | | | | | | | | | | | S | | | | | | |

FIGURE 4

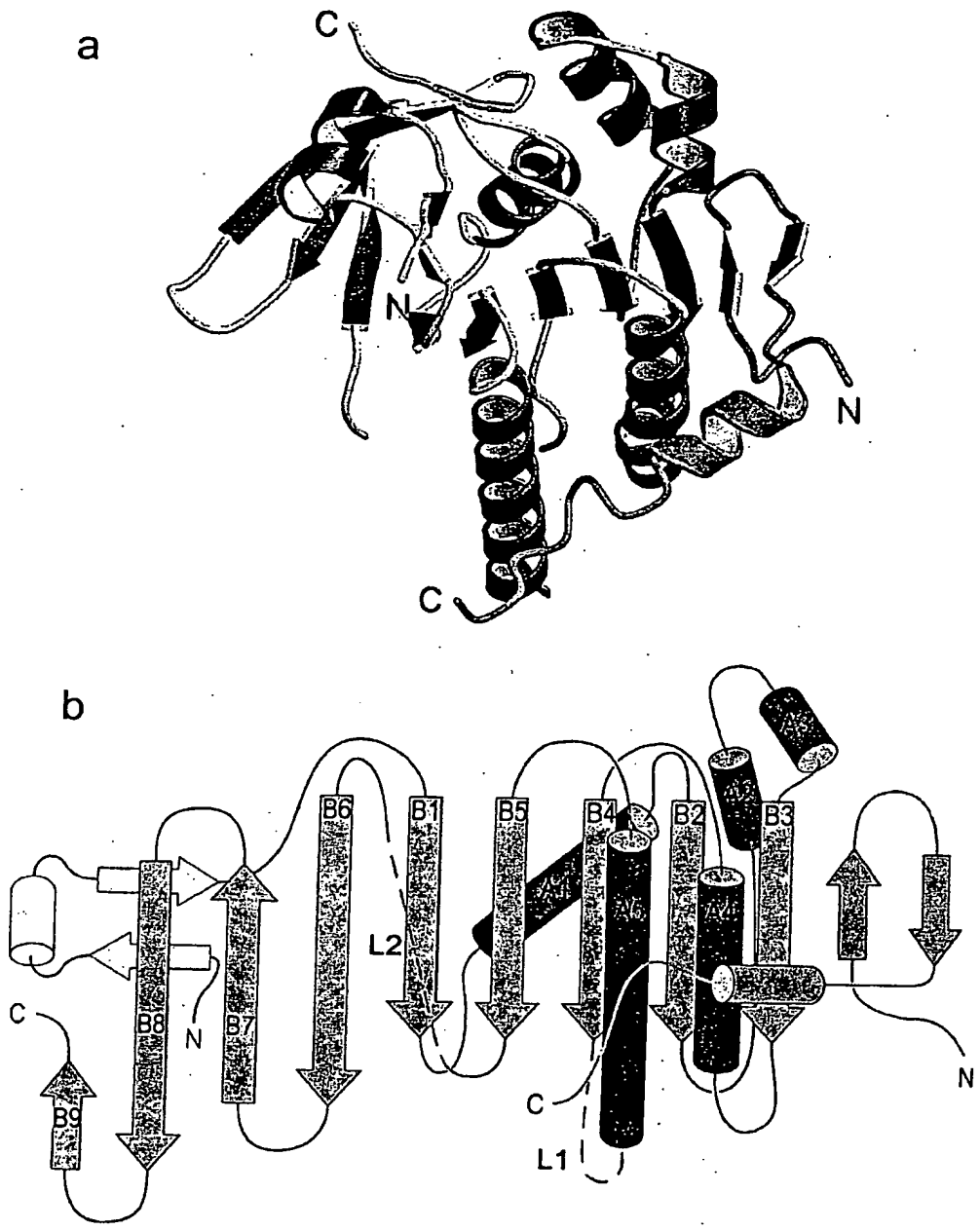


FIGURE 5

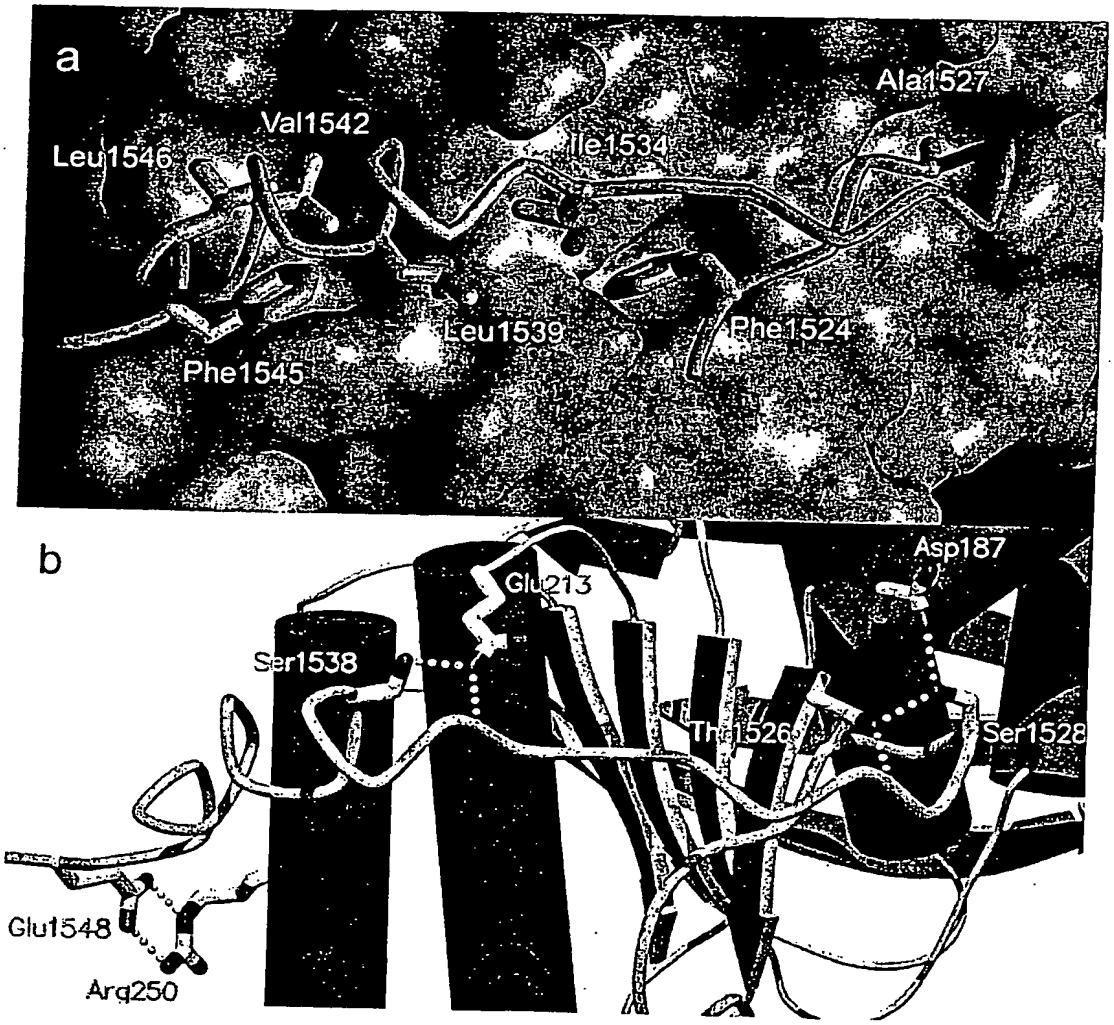
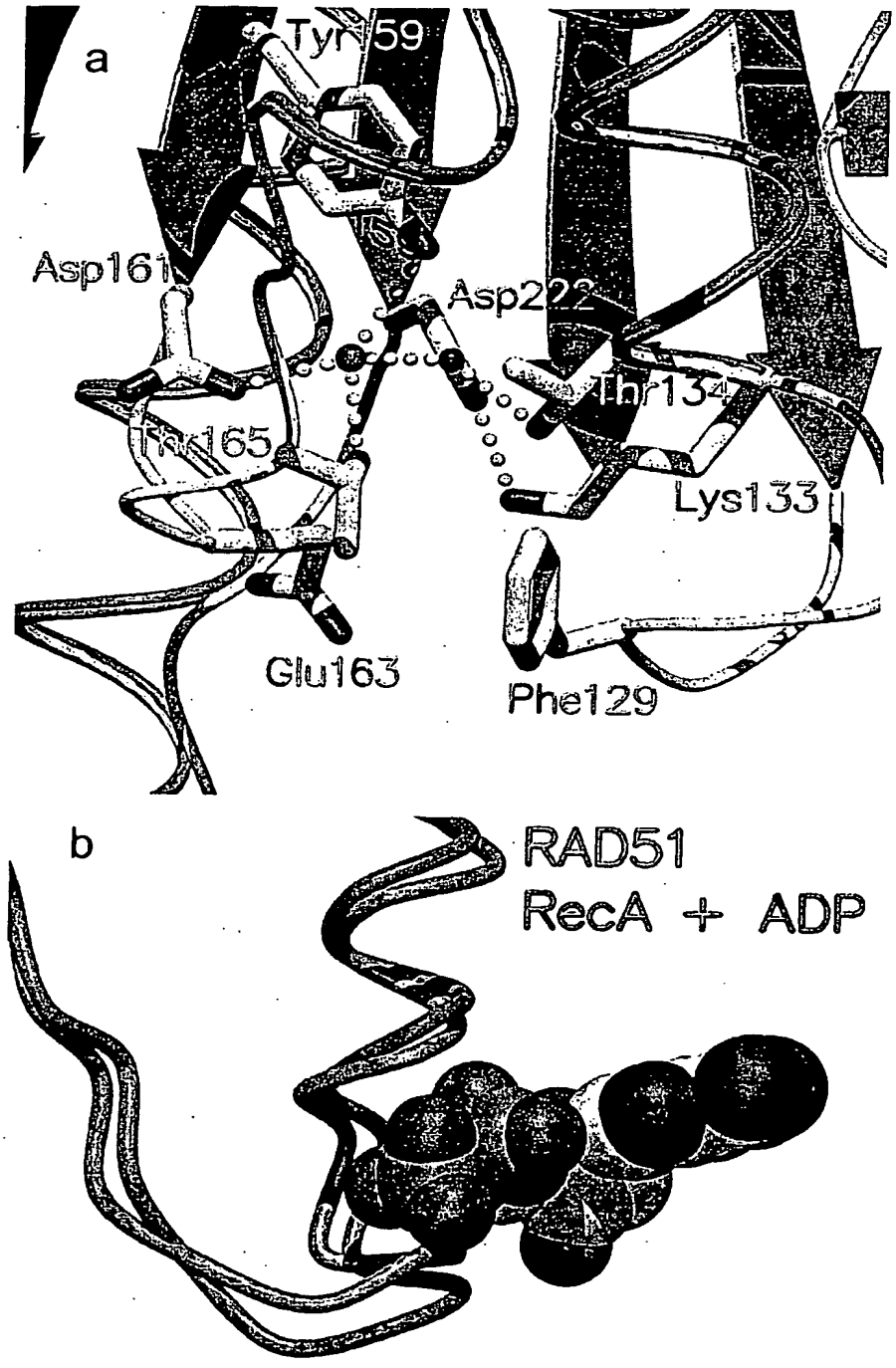
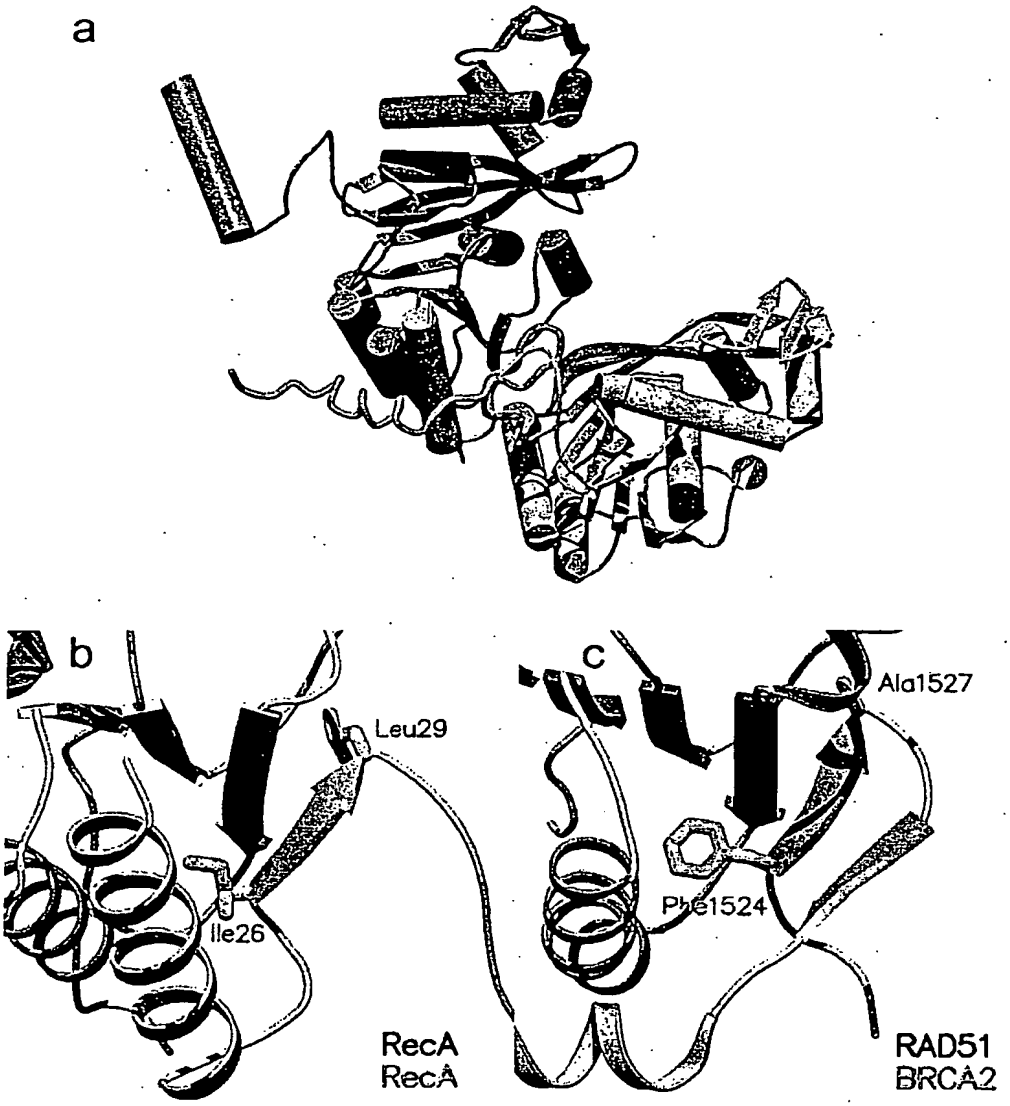


FIGURE 6




Venkitaraman_fig3

FIGURE 7




d

| | | | |
|---|---|---|---|
| RAD51 | H. sapiens | 85-G | F T T A T E-91 |
| " | C. griseus | 85-G | F T T A T E-91 |
| " | X. laevis | 82-G | F T T A T E-88 |
| " | D. melanogaster | 82-G | F L S A R T-88 |
| " | S. cerevisiae | 143-G | F V T A A D-149 |
| DMC1 | H. sapiens | 85-G | F L T A F E-91 |
| RADA | P. furiosus | 95-T | F M R A D E-102 |
| RecA | E. coli | 25-S | I M R L G E-31 |
| BRCA2 | BRC4 H. sapiens | 1523-G | F H T A S G-1529 |

FIGURE 8

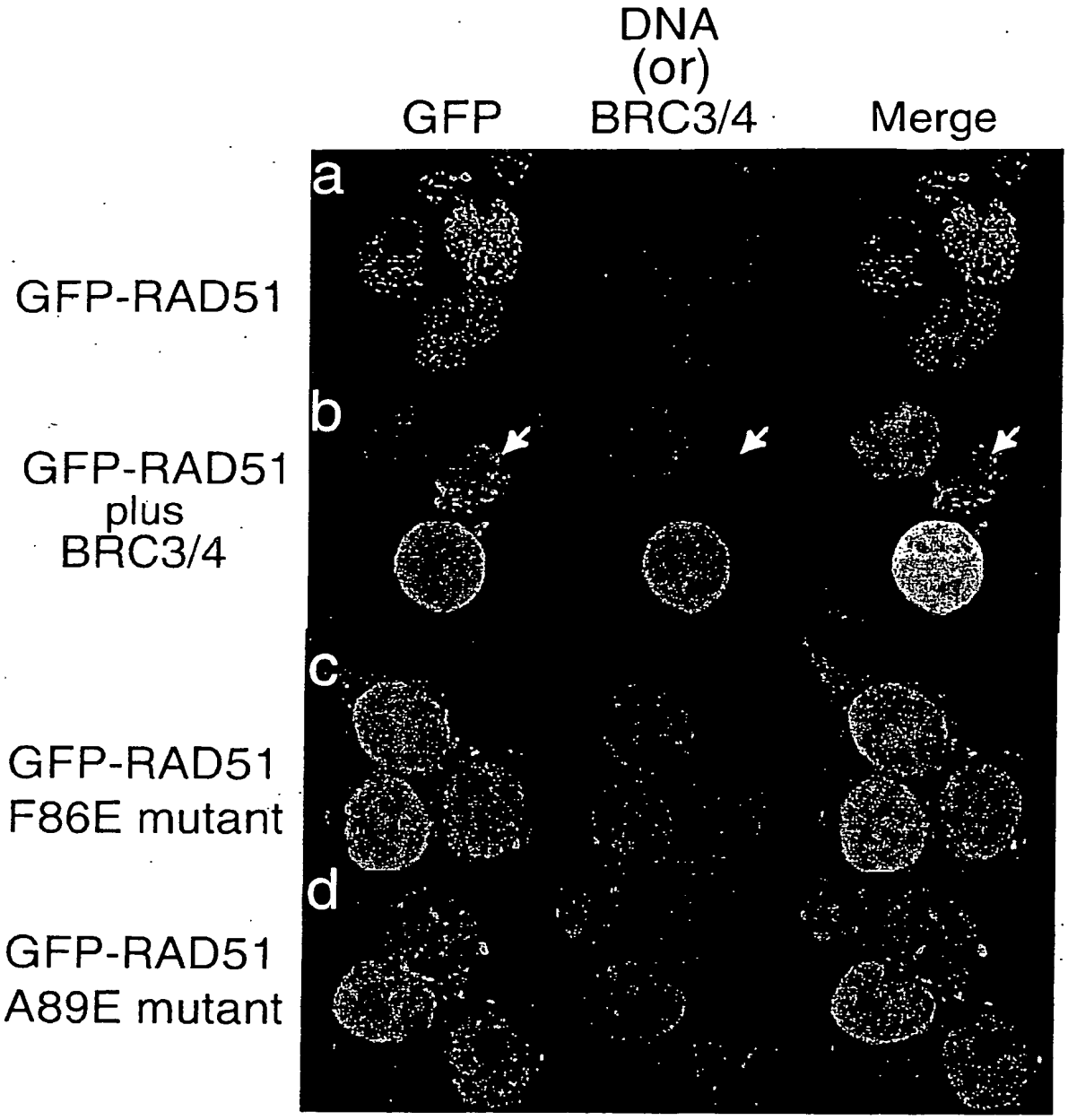


Figure 9(a)

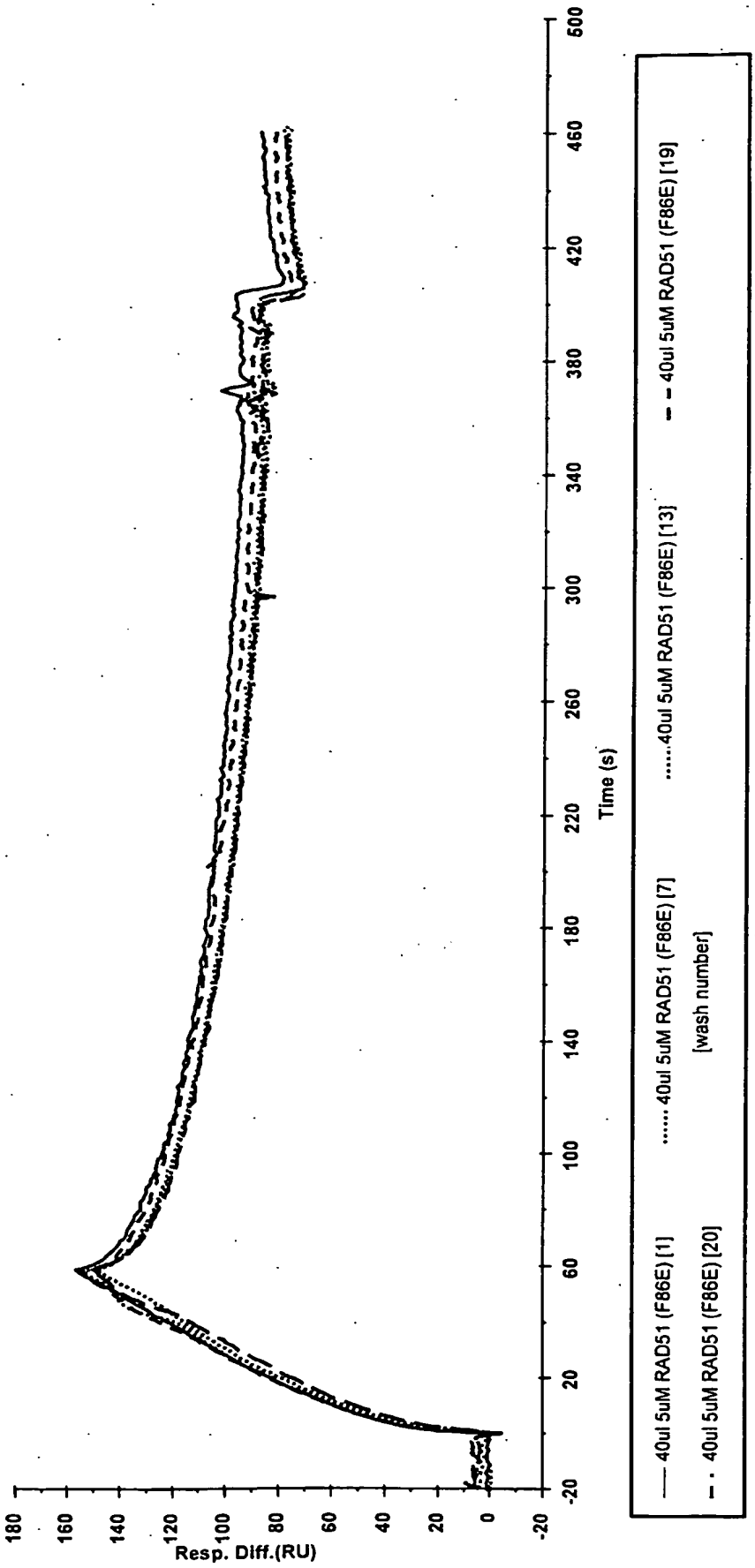

Resp. Diff.(RU)
180
160
140
120
100
80
60
40
20
0
-20
Time (s)
-20
20
60
100
140
180
220
260
300
340
380
420
460
500
40ul 5uM RAD51 (F86E) [1]
40ul 5uM RAD51 (F86E) [7]
40ul 5uM RAD51 (F86E) [13]
40ul 5uM RAD51 (F86E) [19]
40ul 5uM RAD51 (F86E) [20]
[wash number]

Figure 9(b)

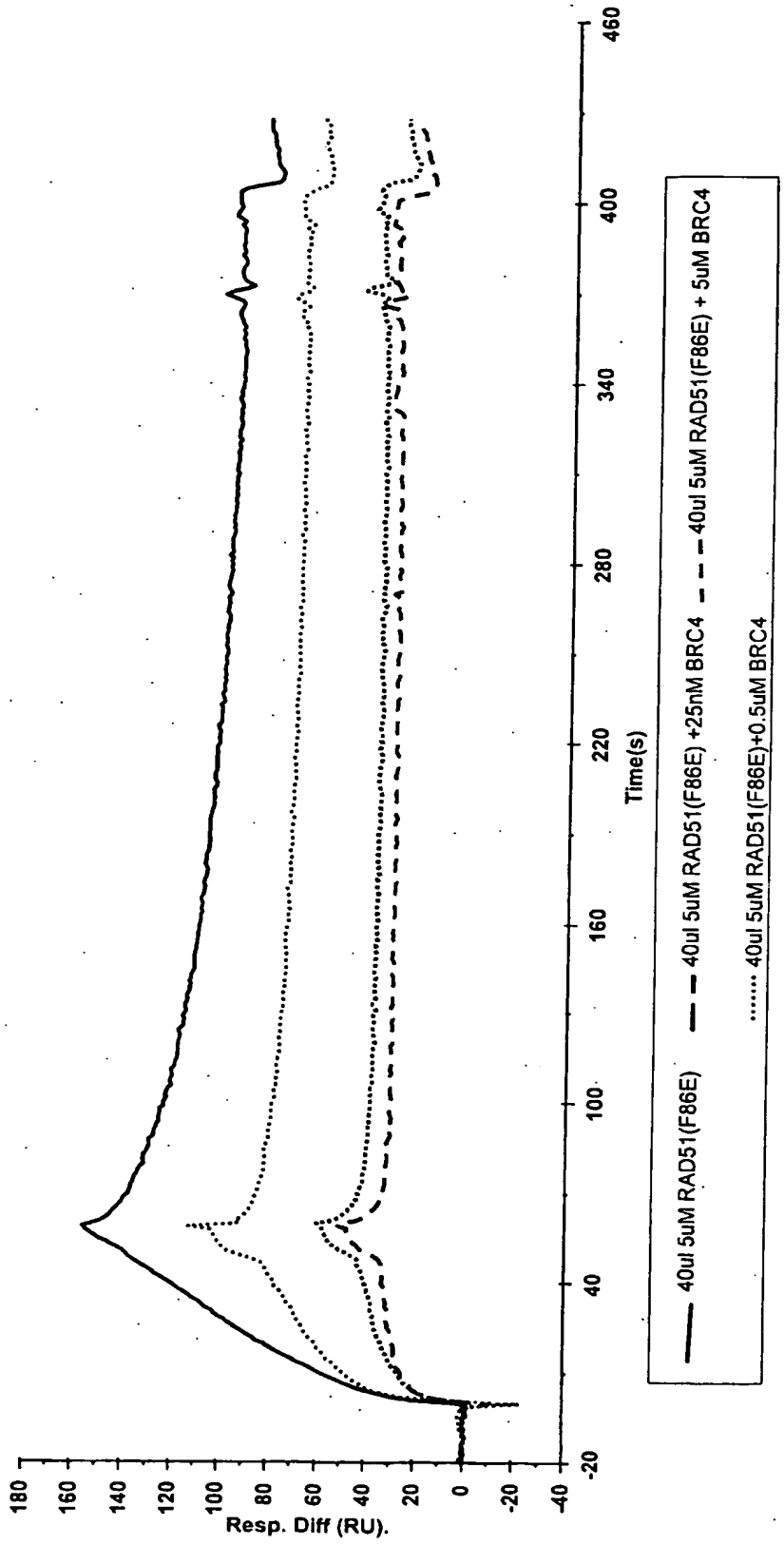
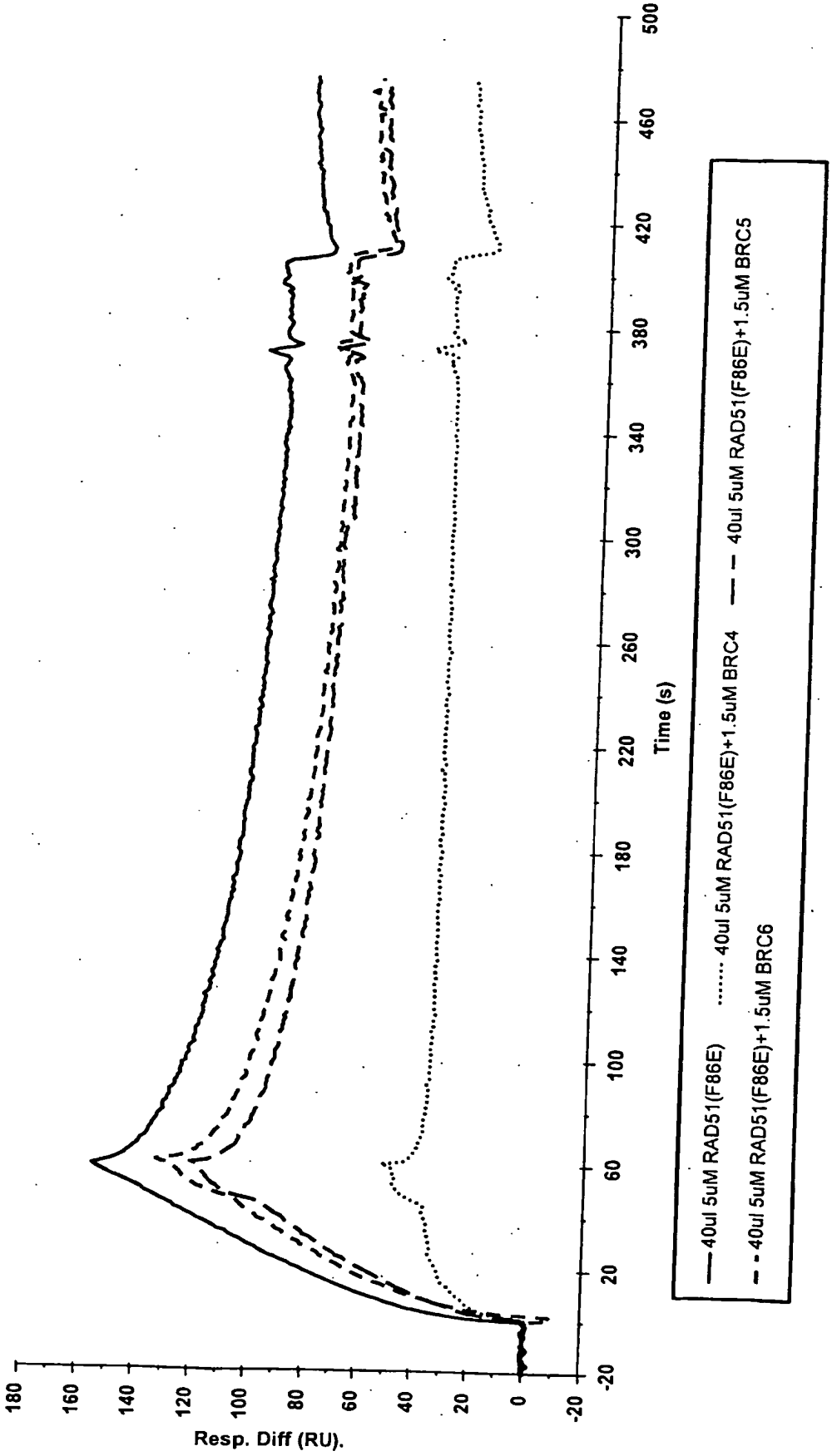

Resp. Diff (RU).
180
160
140
120
100
80
60
40
20
0
-20
-40
Time(s)
-20
40
100
160
220
280
340
400
460
40ul 5uM RAD51(F86E)
40ul 5uM RAD51(F86E) +25nM BRC4
40ul 5uM RAD51(F86E) + 5uM BRC4
40ul 5uM RAD51(F86E)+0.5uM BRC4

Figure 9(c)


Resp. Diff (RU).
180
160
140
120
100
80
60
40
20
0
-20
Time (s)
-20
20
60
100
140
180
220
260
300
340
380
420
460
500
40ul 5uM RAD51(F86E)
40ul 5uM RAD51(F86E)+1.5uM BRC4
40ul 5uM RAD51(F86E)+1.5uM BRC5
40ul 5uM RAD51(F86E)+1.5uM BRC6